Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Synthesis of 3,4,5-trisubstituted isoxazoles via 1,3-dipolar cycloaddition/SO_2 extrusion of benzoisothiazole-2,2- dioxide-3-ylidenes with nitrile oxides

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General

All the reagents were purchased from TCI chemicals and local suppliers and used without purification. The starting materials **1** were prepared following our previous paper[1]. All reactions were monitored by TLC. Chromatography refers to open column chromatography on silica gel (100-200 mesh).

^{1}H NMR spectra were recorded on 500 MHz and ^{13}C NMR spectra were recorded on 125 MHz by using a Bruker Avance 500M spectrometer. Chemical shifts were reported in parts per million (δ) relative to tetramethylsilane (TMS). Mass spectra were performed on an Ultima Global spectrometer with an ESI source. The X-ray single-crystal diffraction was performed on Saturn 724+ instrument.

General procedure for the preparation of 3,4,5-trisubstituted isoxazoles 4

To a mixture of (*Z*)-benzoisothiazole-2,2-dioxide-3-ylidenes **1** (0.2 mmol) and powdered 4Å MS (0.11g, 0.6 mmol) in toluene (1 mL), nitrile oxide precursors **2** (0.6 mmol) was added slowly during 24 thours. After that, the mixture was filtered and the filtrate was evaporated to remove solvent under reduced pressure.. The residue was subjected to column chromatography on silica gel (100-200 mesh) using petroleum/dichloromethane as eluent to afford dipolarophiles **4**.

{2-[3-(4-Methoxy-phenyl)-4-phenyl-isoxazol-5-yl]-phenyl}-methyl-amine (4o) (CCDC 1441667)

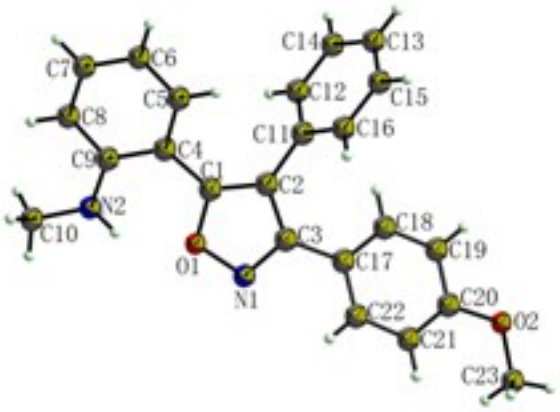
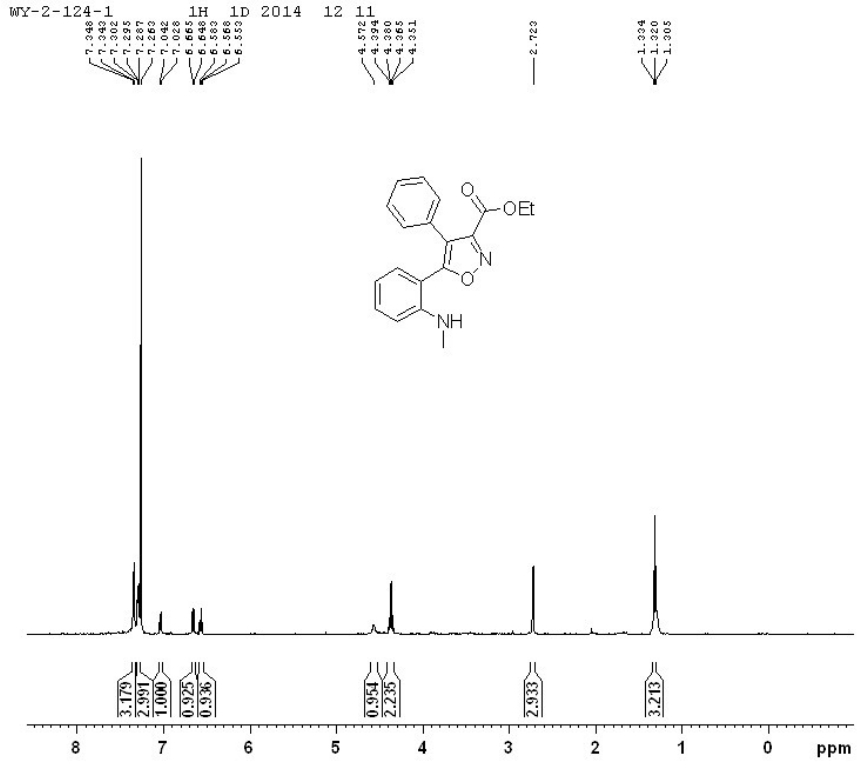


Fig 2. X-ray crystallography of compound **4o**.

1. Cao, G.; Long, F.; Zhao, Y.; Wang, Y.; Huang, L.; Teng D. *Tetrahedron*, **2014**, 70, 9359-9365.

Characterization spectra of compounds 4

^{1}H NMR Spectrum of 4a



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FIDRES	0.610352 Hz
AQ	0.8193000 sec
RG	575
DW	50.000 usec
DE	8.00 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
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NUC1	1H
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PL1	2.00 dB
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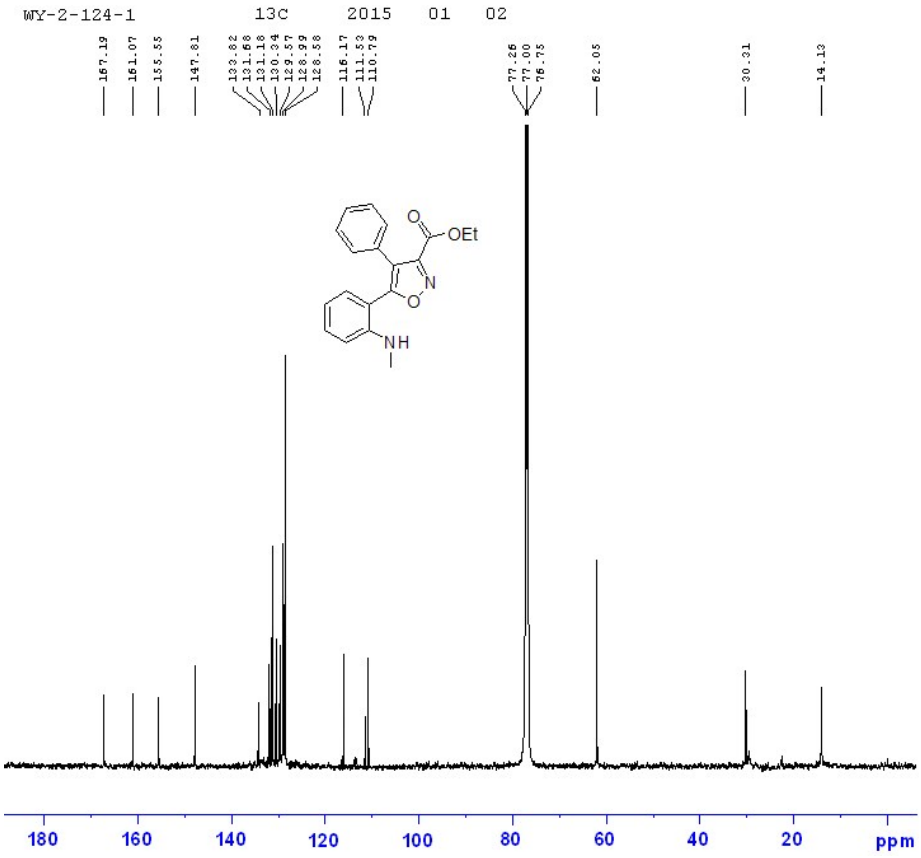
^{13}C NMR Spectrum of 4a



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RG	1820
DW	15.300 usec
DE	6.00 usec
TE	673.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	40
======== CHANNEL f1 ========	
NUC1	13C
P1	12.20 usec
PL1	3.00 dB
SFO1	125.7464750 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	17.70 dB
PL13	17.70 dB
SFO2	500.0355000 MHz
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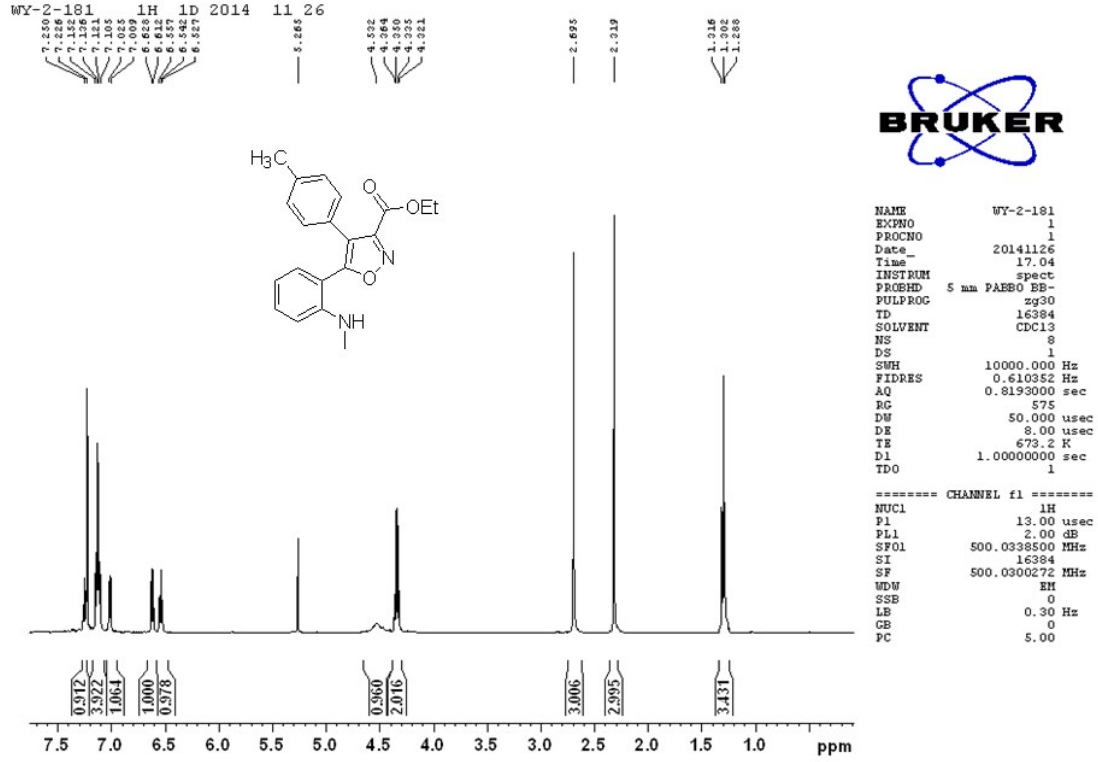
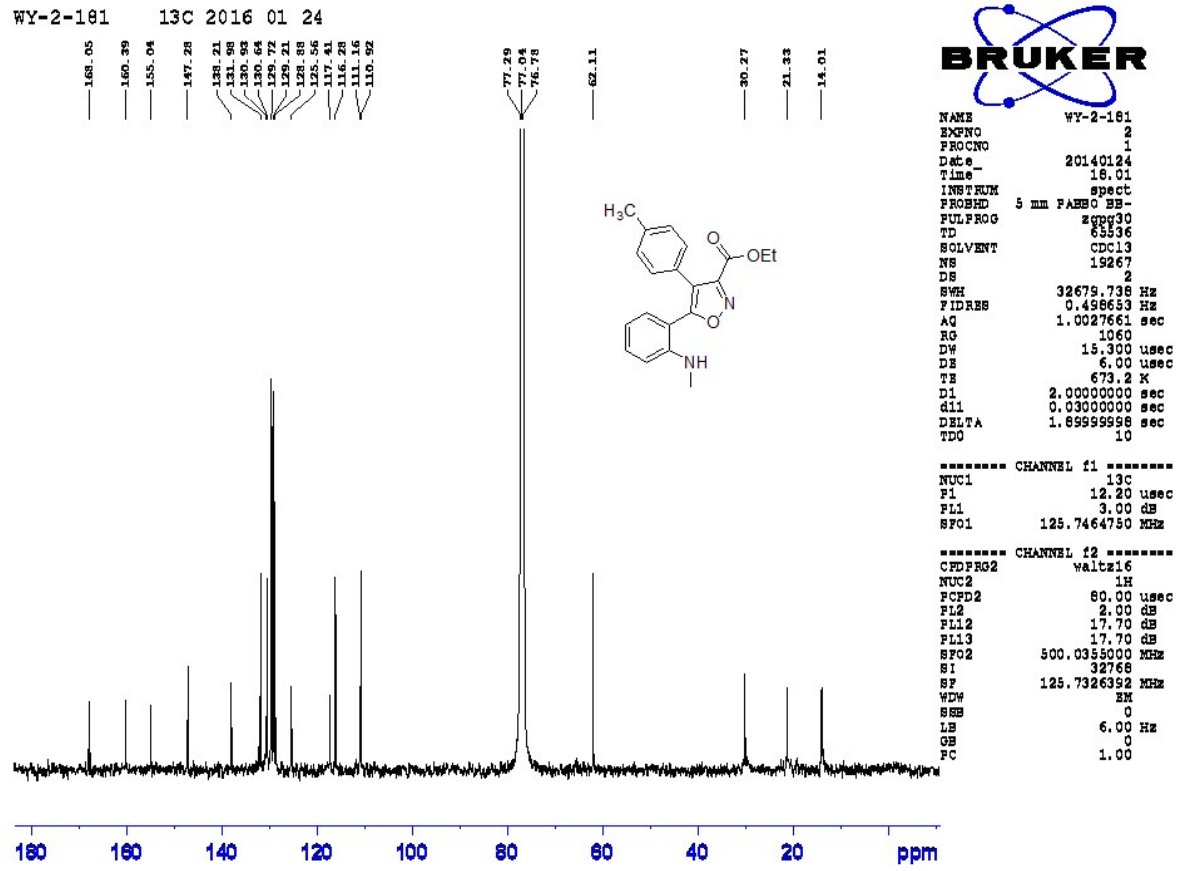
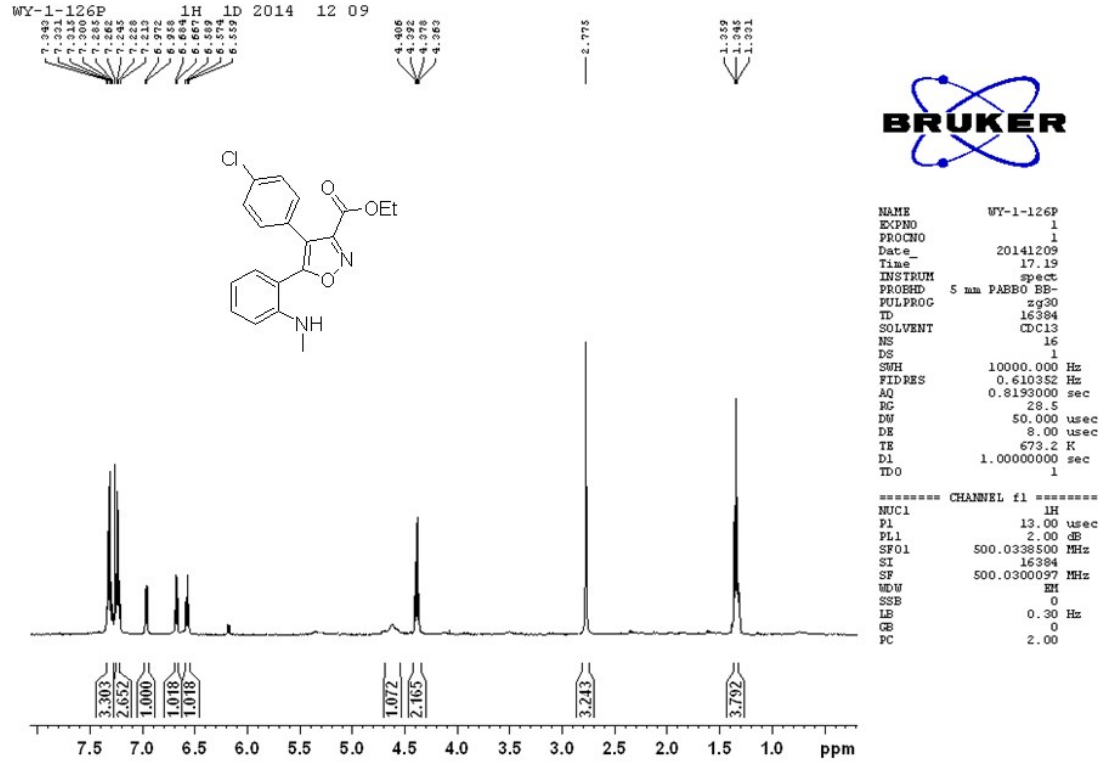
^{1}H NMR Spectrum of 4b



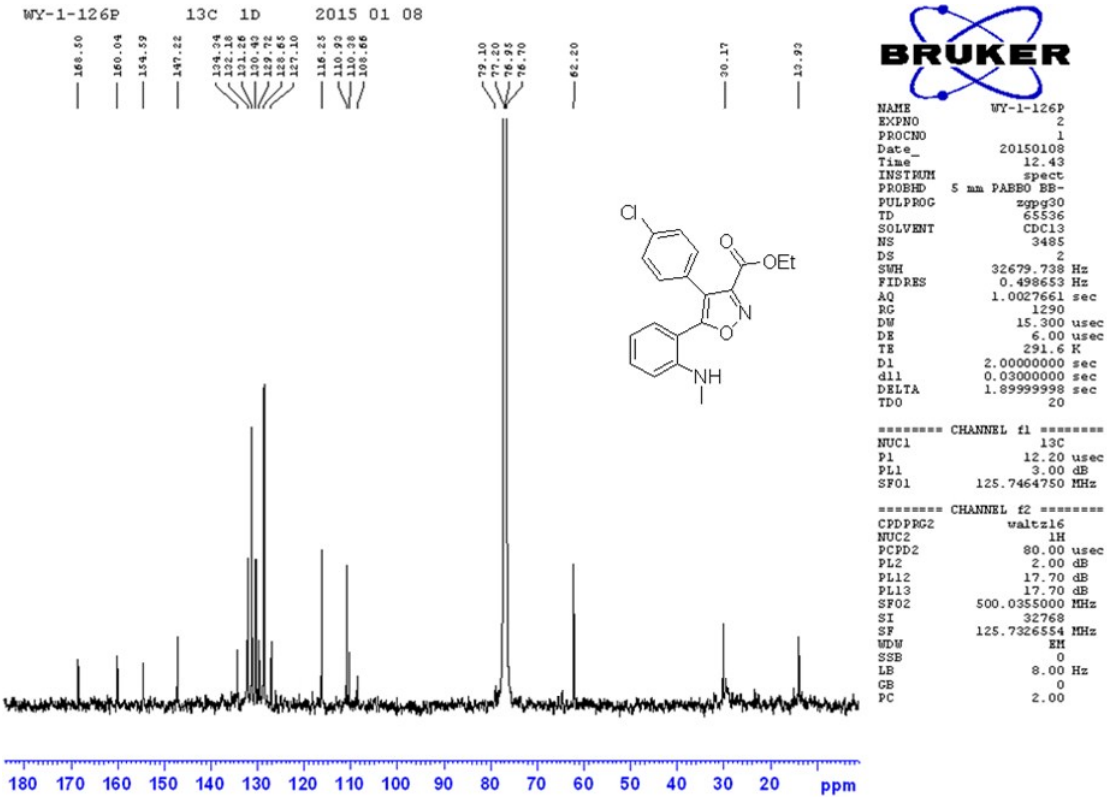
^{13}C NMR Spectrum of 4b



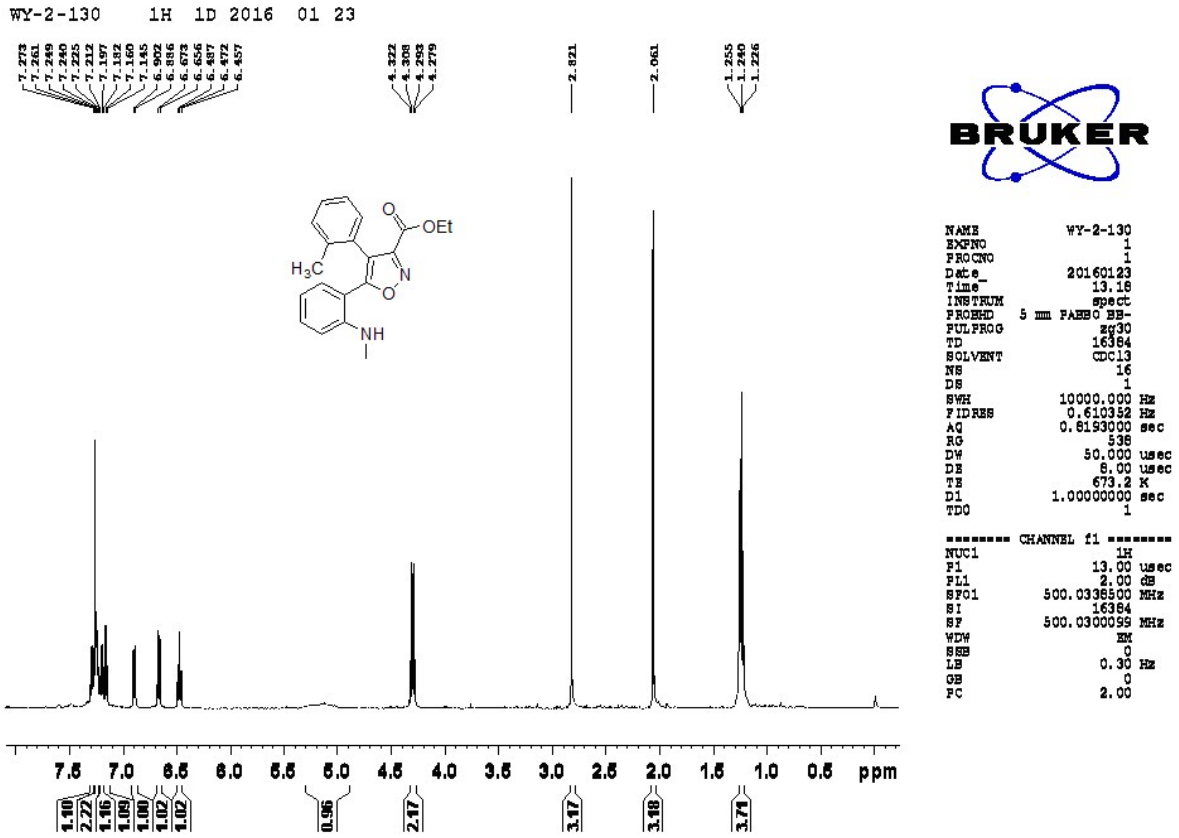
^{1}H NMR Spectrum of 4c



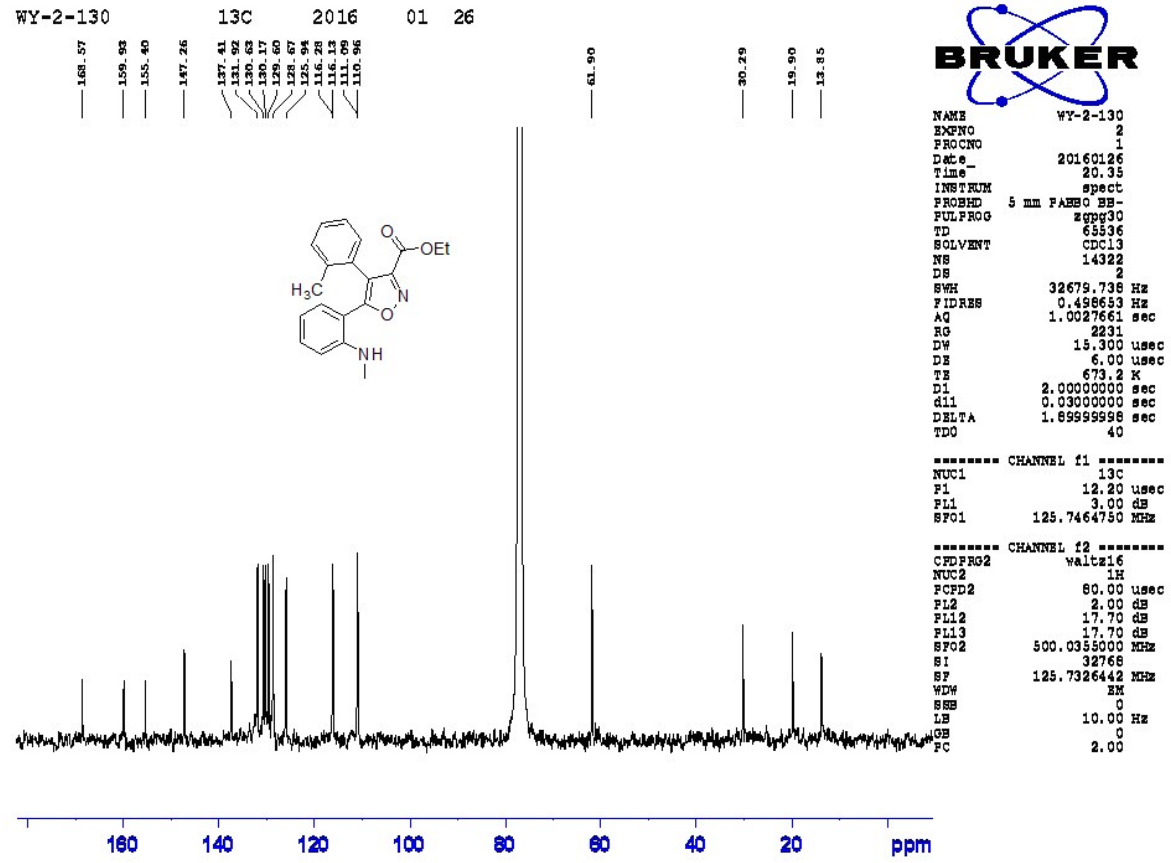
^{13}C NMR Spectrum of 4c



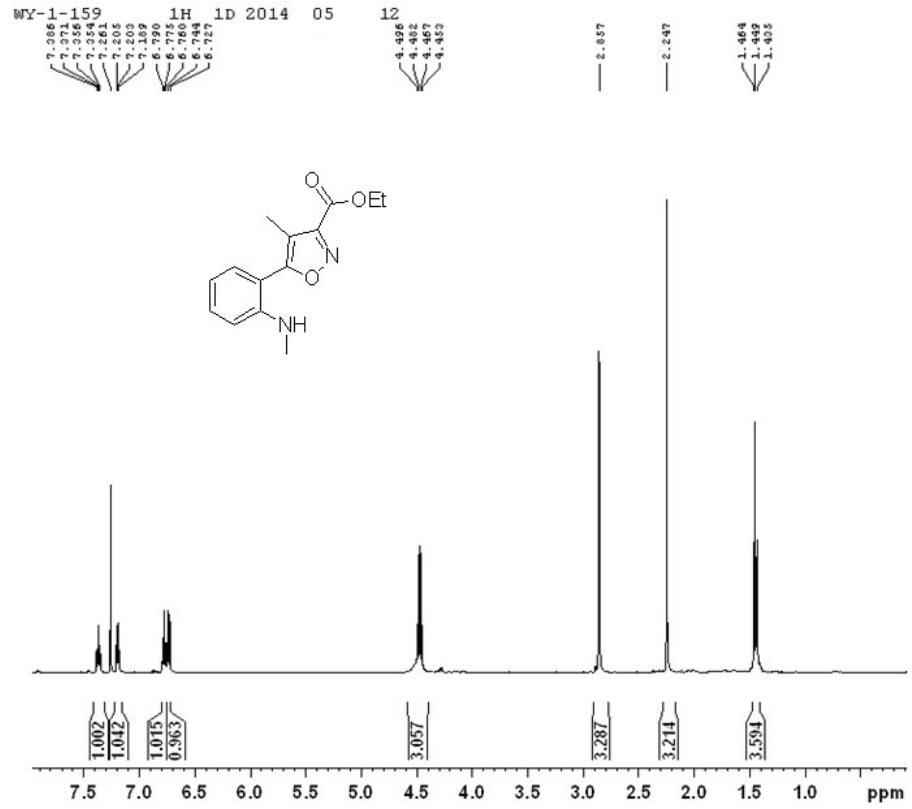
^{1}H NMR Spectrum of 4d



^{13}C NMR Spectrum of 4d



[1]H NMR Spectrum of 4e



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RG	1150
DW	50.000 usec
DE	8.00 usec
TE	297.5 K
D1	1.00000000 sec
TD0	1
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P1	13.00 usec
PL1	2.00 dB
SFO1	500.0338500 MHz
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SSB	0
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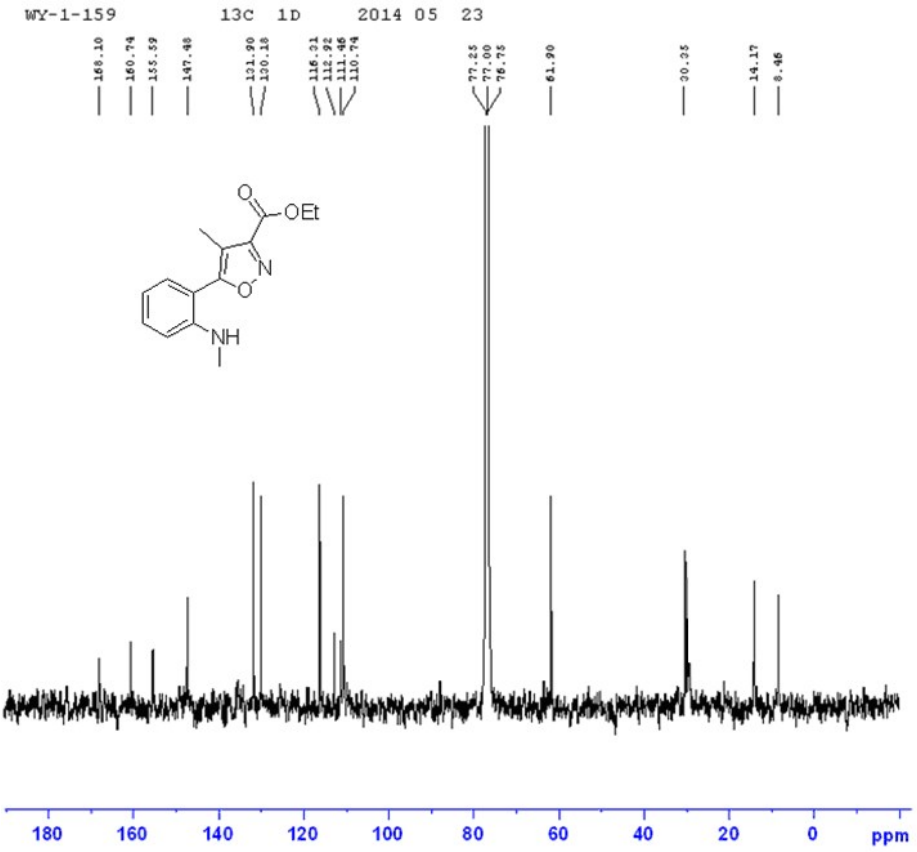
PC	4.00

[13]C NMR Spectrum of 4e



BRUKER

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PROCNO	1
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FIDRES	0.498653 Hz
AQ	1.0027661 sec
RG	1820
DW	15.300 usec
DE	6.00 usec
TE	299.3 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	20
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NUC1	13C
P1	12.20 usec
PL1	3.00 dB
SFO1	125.7464750 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	17.70 dB
PL13	17.70 dB
SFO2	500.0355000 MHz
SI	32768
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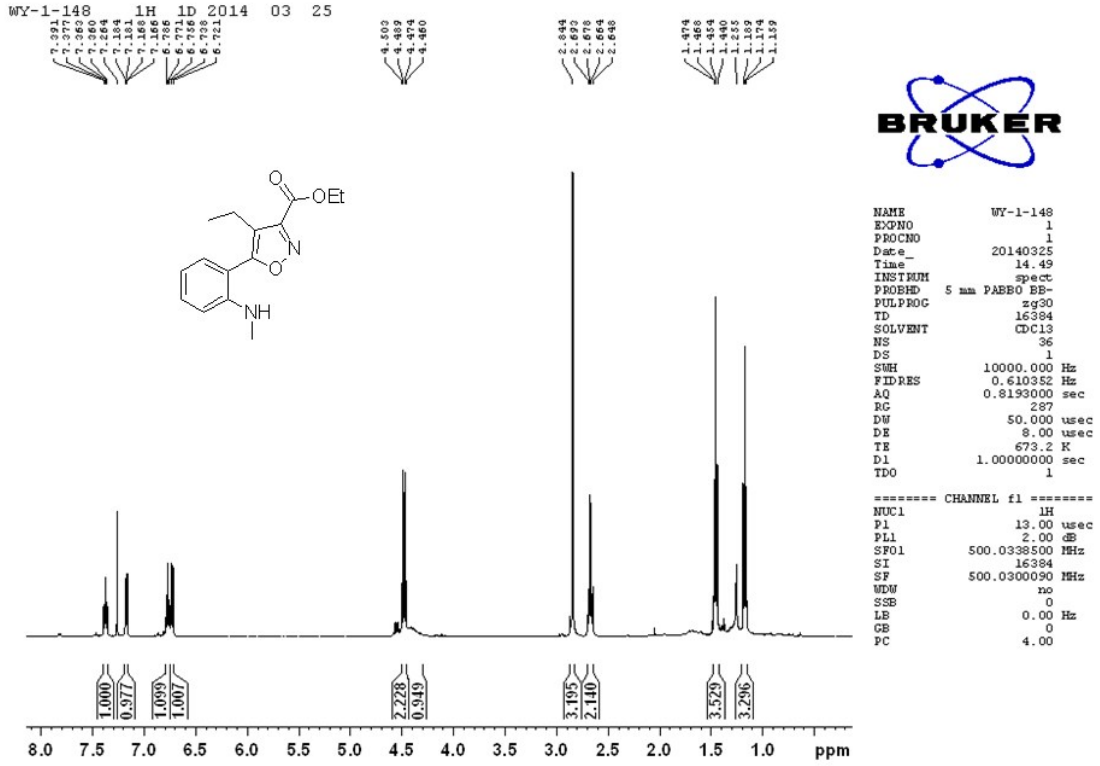
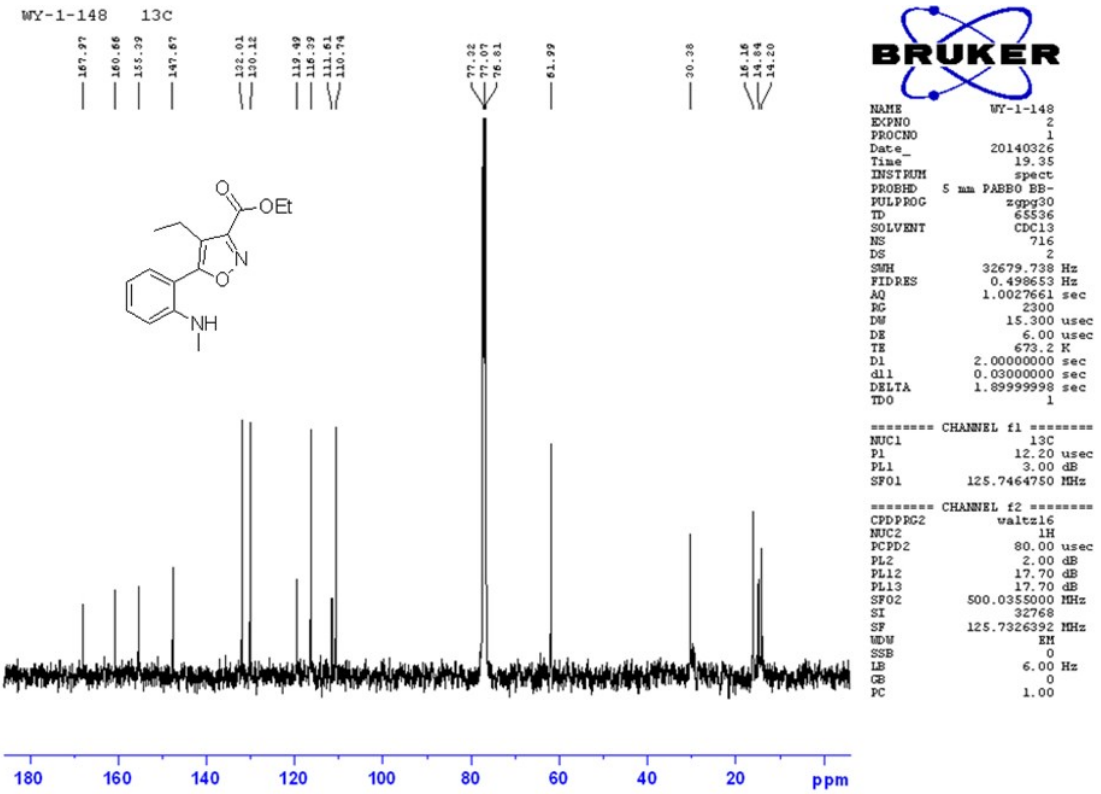
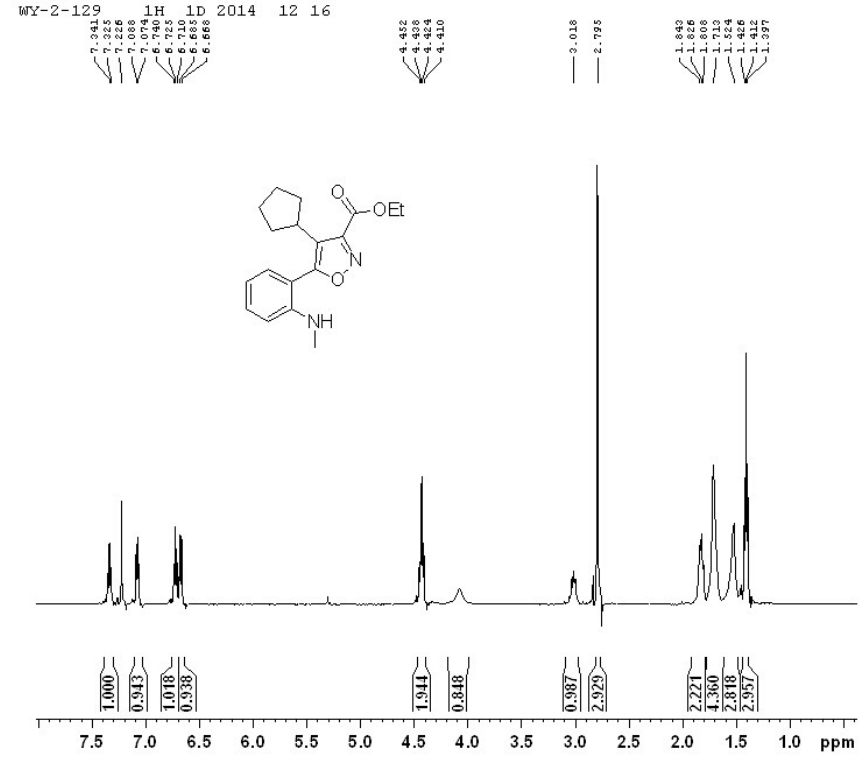
^{1}H NMR Spectrum of 4f



^{13}C NMR Spectrum of 4f



^{1}H NMR Spectrum of 4g



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FIDRES	0.610352 Hz
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RG	18
DW	50.000 usec
DE	8.00 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
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PL1	2.00 dB
SFO1	500.0338500 MHz
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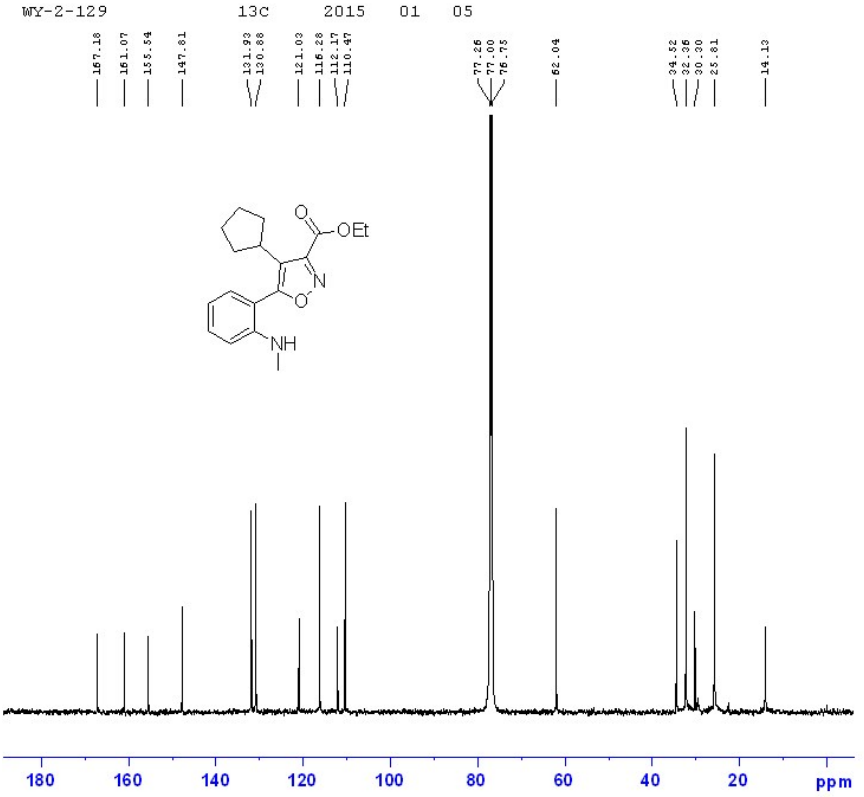
^{13}C NMR Spectrum of 4g



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FIDRES	0.498653 Hz
AQ	1.0027661 sec
RG	3250
DW	15.300 usec
DE	6.00 usec
TE	673.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	40
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NUC1	13C
P1	12.20 usec
PL1	3.00 dB
SFO1	125.7464750 MHz
========	CHANNEL f2 ========
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	17.70 dB
PL13	17.70 dB
SFO2	500.0355000 MHz
SI	32768
SF	125.7326440 MHz
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SSB	0
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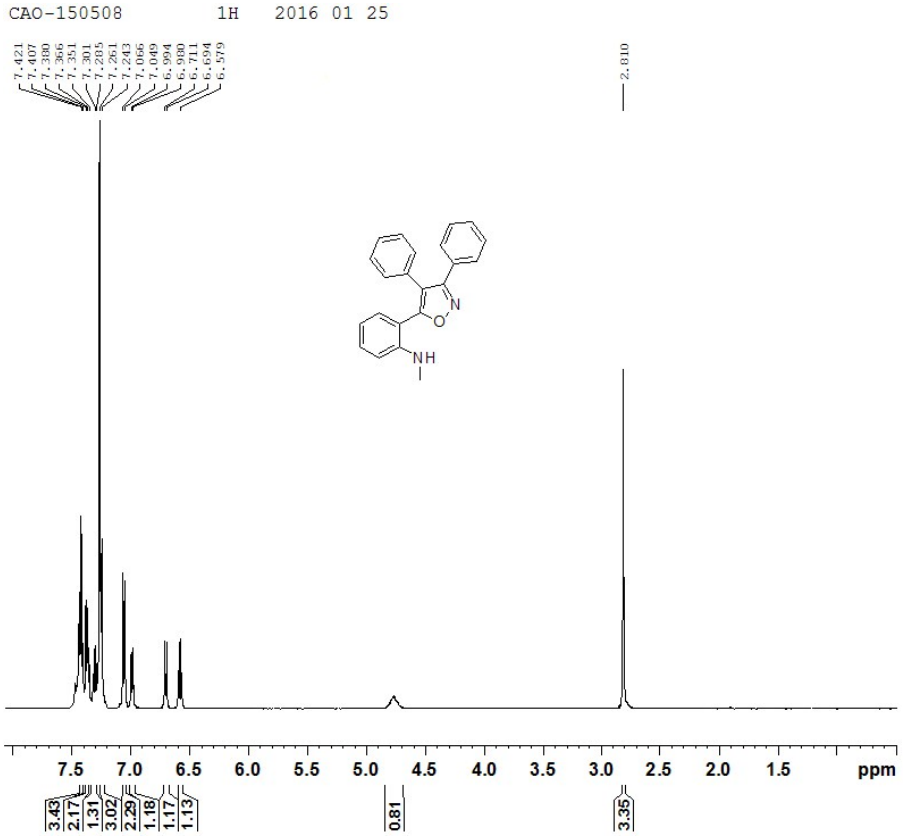
PC	2.00

^{1}H NMR Spectrum of 4k

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TD                 32768
SOLVENT            CDC13
NS                    16
DS                     1
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FIDRES        0.305176 Hz
AQ            1.6385000 sec
RG                   907
DW                50.000 usec
DE                 6.00 usec
TE                673.2 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  1H
P1                 13.00 usec
PL1                 2.00 dB
SFO1         500.0335010 MHz
SI                 16384
SF           500.0300101 MHz
WDW                   EM
SSB                    0
LB                  0.30 Hz
GB                     0
PC                  4.00
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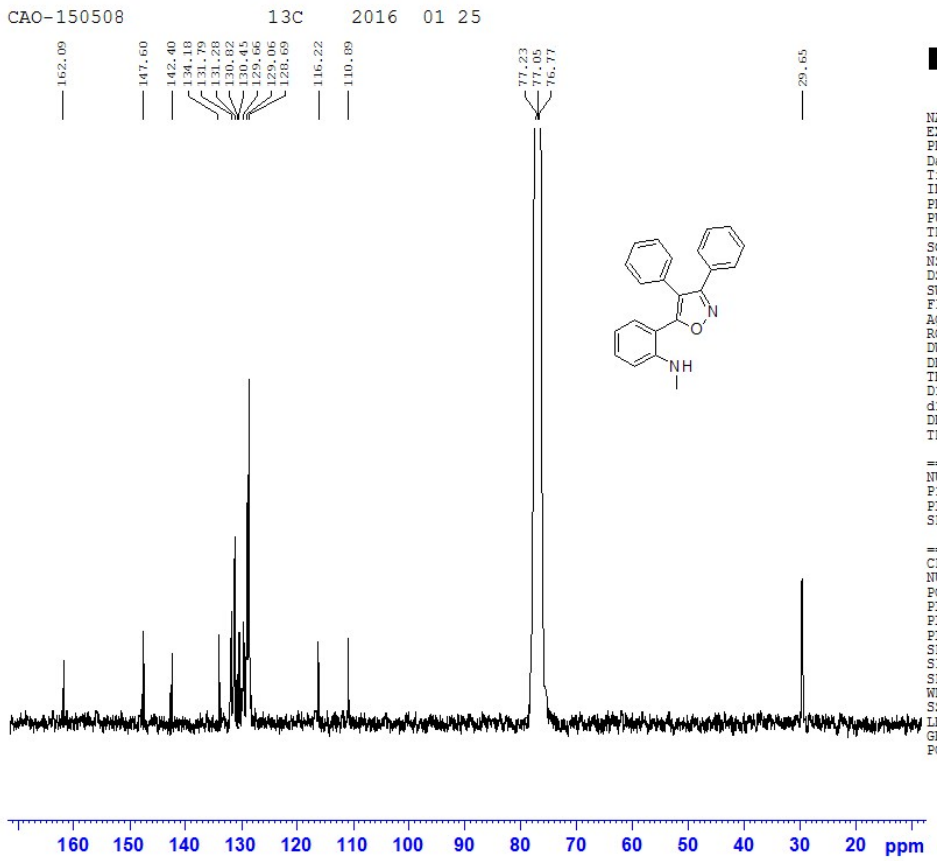
^{13}C NMR Spectrum of 4k

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FIDRES        0.498653 Hz
AQ            1.0027661 sec
RG                   533
DW                15.300 usec
DE                 6.00 usec
TE                673.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                   20

======== CHANNEL f1 ========
NUC1                 13C
P1                 12.20 usec
PL1                 3.00 dB
SFO1         125.7464750 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                  1H
PCPD2              80.00 usec
PL2                 2.00 dB
PL12               17.70 dB
PL13               17.70 dB
SFO2         500.0355000 MHz
SI                 32768
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WDW                   EM
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PC                  1.00
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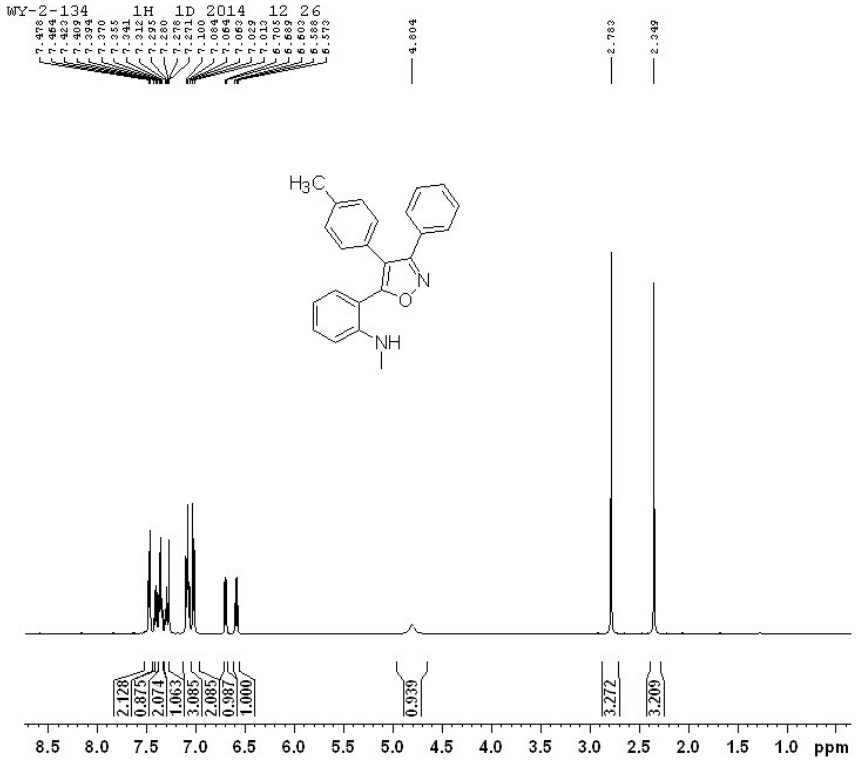
^{1}H NMR Spectrum of 4l



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AQ	0.8193000 sec
RG	406
DW	50.000 usec
DE	8.00 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
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P1	13.00 usec
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SF01	500.0338500 MHz
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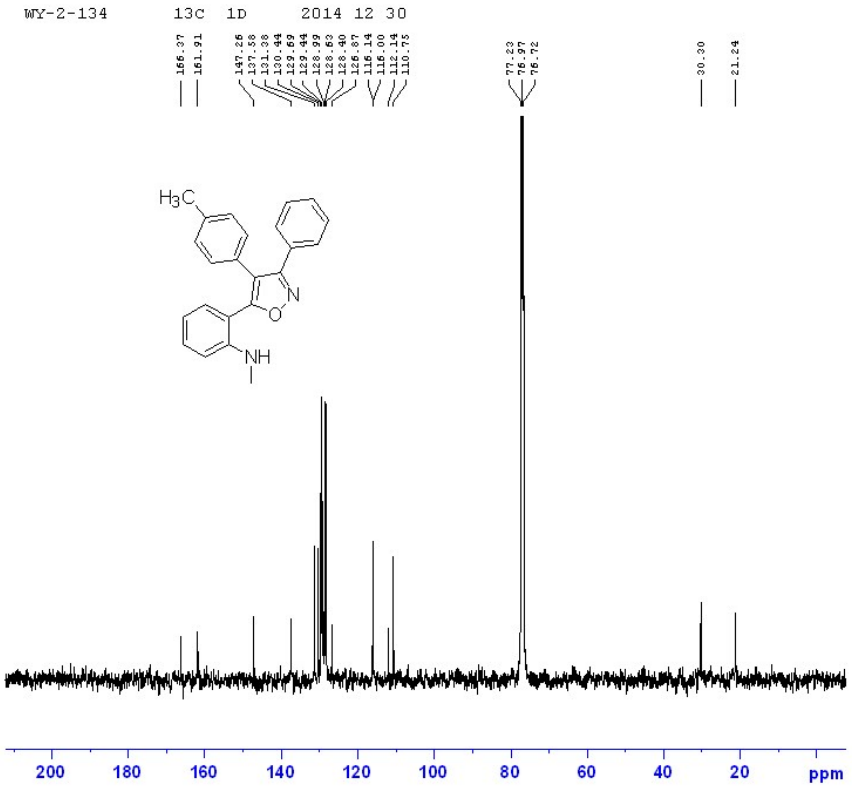
PC	2.00

^{13}C NMR Spectrum of 4l



BRUKER

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FIDRES	0.498653 Hz
AQ	1.0027661 sec
RG	2890
DW	15.300 usec
DE	6.00 usec
TE	673.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	20
======== CHANNEL f1 ========	
NUC1	13C
P1	12.20 usec
PL1	3.00 dB
SF01	125.7464750 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	17.70 dB
PL13	17.70 dB
SF02	500.0355000 MHz
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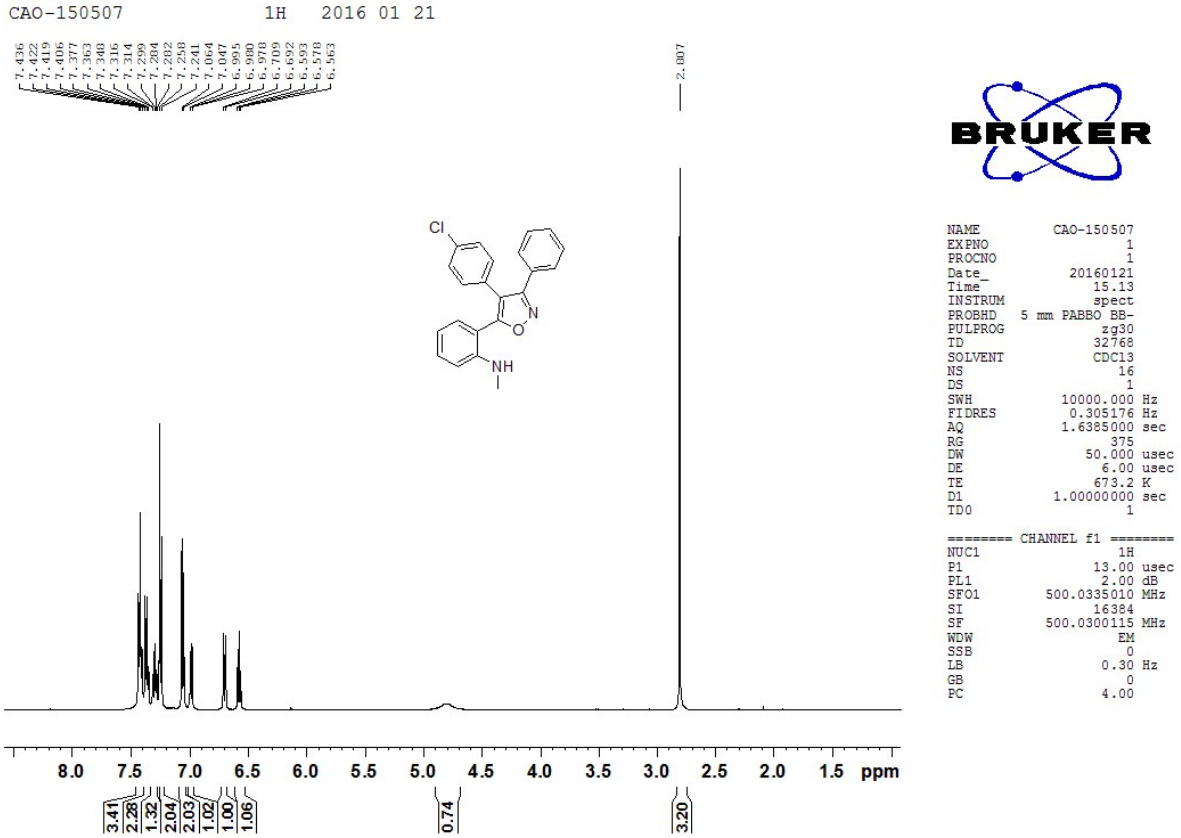
PC	4.00

^{1}H NMR Spectrum of 4m



BRUKER

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AQ	1.6385000 sec
RG	375
DW	50.000 usec
DE	6.00 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.00 usec
PL1	2.00 dB
SFO1	500.0335010 MHz
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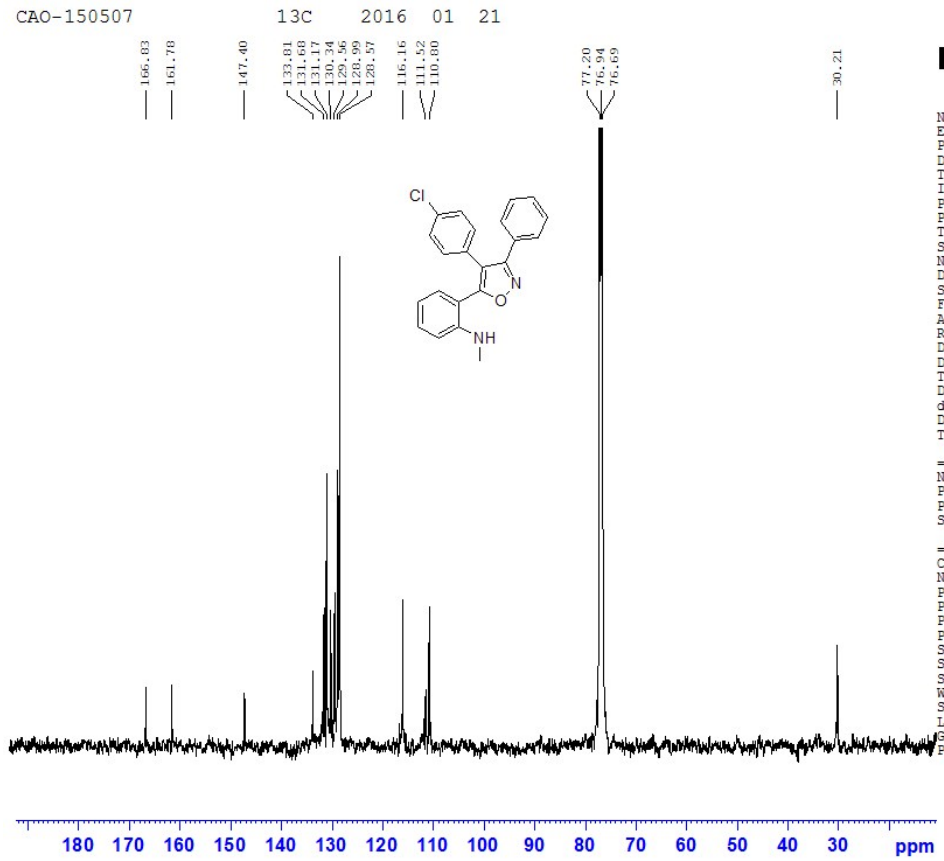
^{13}C NMR Spectrum of 4m



BRUKER

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FIDRES	0.498653 Hz
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RG	435
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DE	6.00 usec
TE	299.1 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	20
======== CHANNEL f1 ========	
NUC1	13C
P1	12.20 usec
PL1	3.00 dB
SFO1	125.7464750 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	17.70 dB
PL13	17.70 dB
SFO2	500.0355000 MHz
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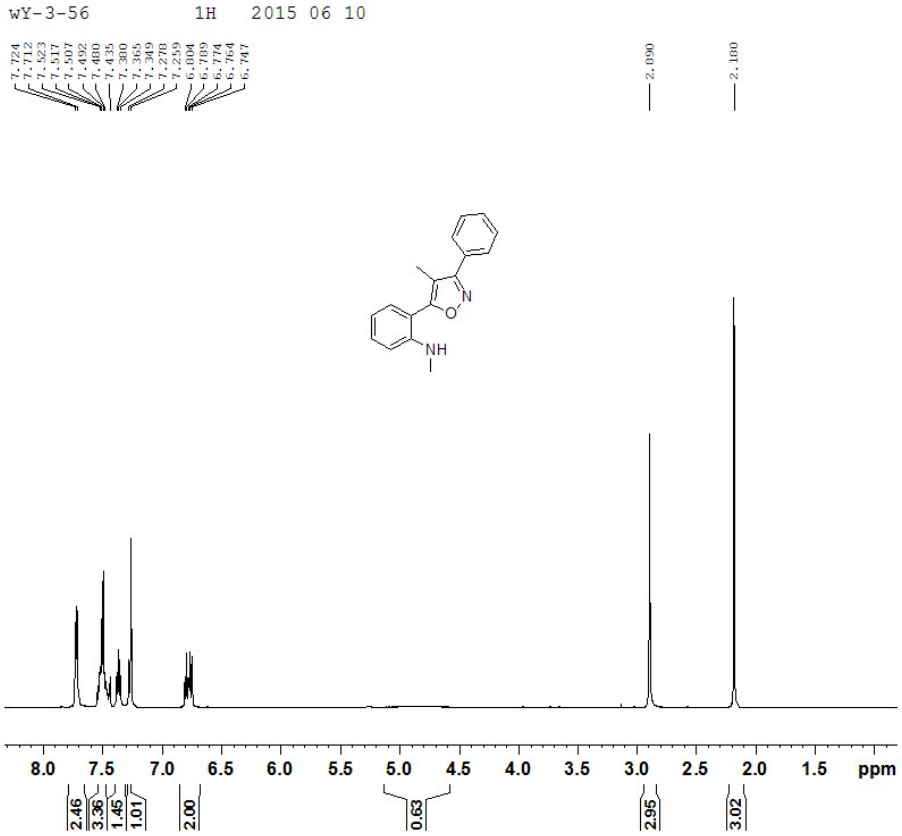
SSB	0
LB	10.00 Hz
GB	0
PC	1.00

^{1}H NMR Spectrum of 4n

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TD                32768
SOLVENT           CDCl3
NS                   16
DS                    1
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            1.6385000 sec
RG                  362
DW             50.000 usec
DE              6.00 usec
TE                298.6 K
D1          1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1               13.00 usec
PL1               2.00 dB
SFO1        500.0335010 MHz
SI                16384
SF          500.0300113 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                4.00
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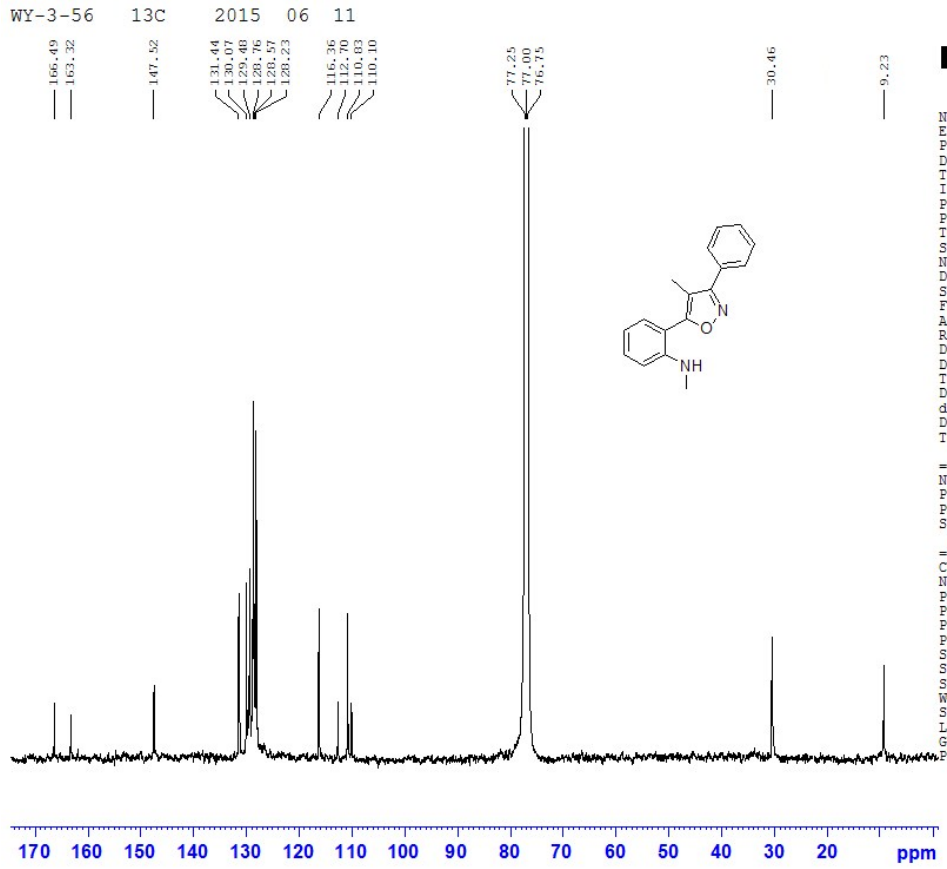
^{13}C NMR Spectrum of 4n

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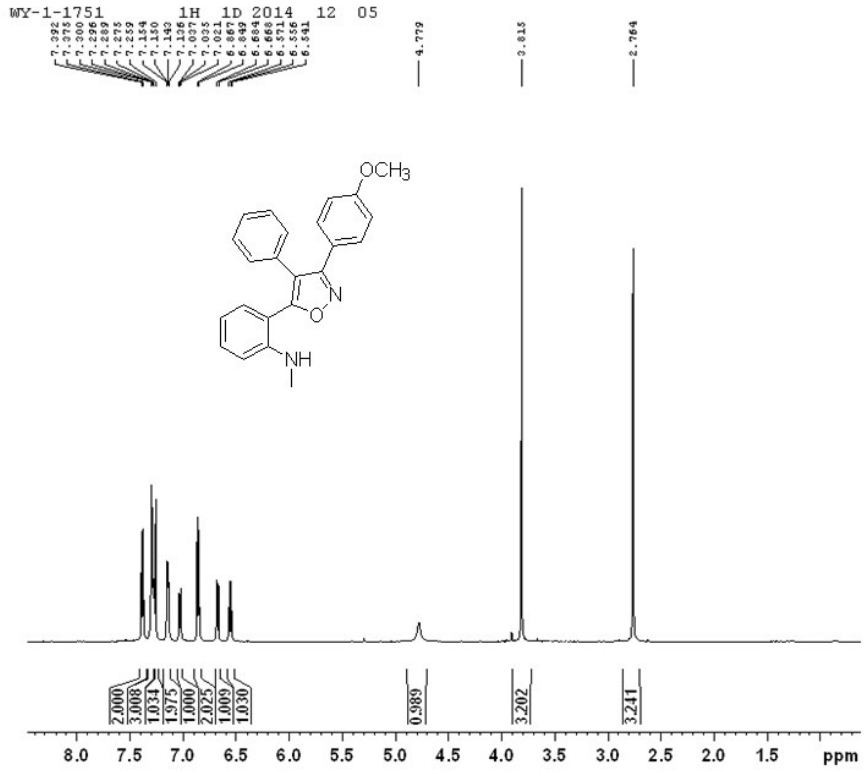
SOLVENT           CDCl3
NS                13894
DS                    2
SWH          32679.738 Hz
FIDRES        0.498653 Hz
AQ            1.0027661 sec
RG                 1820
DW             15.300 usec
DE              6.00 usec
TE                673.2 K
D1          2.00000000 sec
d11         0.03000000 sec
DELTA       1.89999998 sec
TD0                  40

======== CHANNEL f1 ========
NUC1                13C
P1               12.20 usec
PL1               3.00 dB
SFO1        125.7464750 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2                 1H
PCPD2            80.00 usec
PL2               2.00 dB
PL12             17.70 dB
PL13             17.70 dB
SFO2        500.0355000 MHz
SI                32768
SF          125.7326425 MHz
WDW                  EM
SSB                   0
LB               10.00 Hz
GB                    0
PC                0.50
```

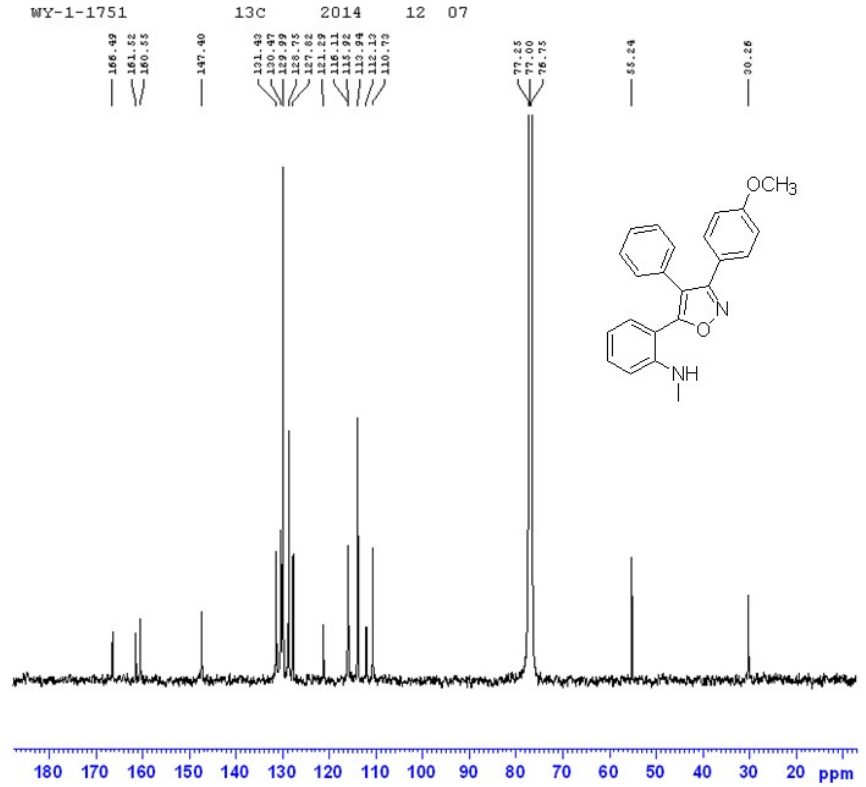
[1]H NMR Spectrum of 4o



BRUKER

NAME	WY-1-1751
EXPNO	1
PROCNO	1
Date_	20141205
Time	15.48
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	16384
SOLVENT	CDCl3
NS	16
DS	1
SWH	10000.000 Hz
FIDRES	0.610352 Hz
AQ	0.8193000 sec
RG	406
DW	50.000 usec
DE	8.00 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.00 usec
PL1	2.00 dB
SF01	500.0338500 MHz
SI	16384
SF	500.0300110 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	0.50

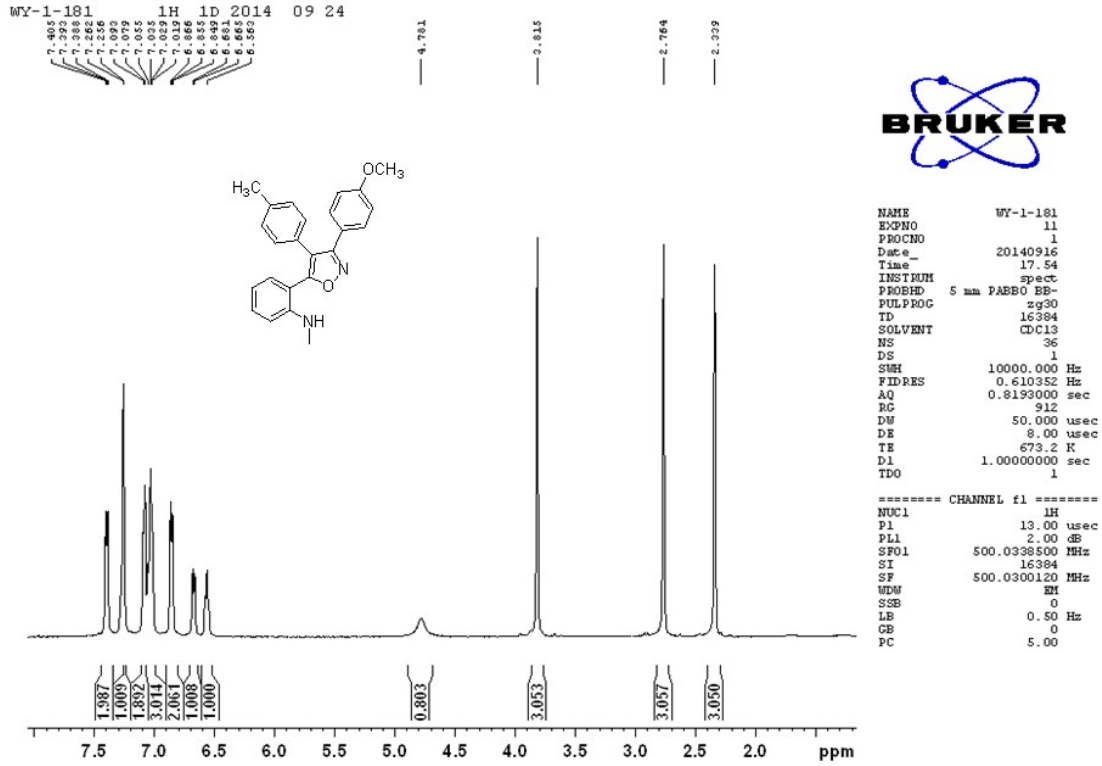
[13]C NMR Spectrum of 4o



BRUKER

NAME	WY-1-1751
EXPNO	2
PROCNO	1
Date_	20141207
Time	12.43
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	3206
DS	2
SWH	32679.738 Hz
FIDRES	0.498653 Hz
AQ	1.0027661 sec
RG	2580
DW	15.300 usec
DE	6.00 usec
TE	673.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	40
======== CHANNEL f1 ========	
NUC1	13C
P1	12.20 usec
PL1	3.00 dB
SF01	125.7464750 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	17.70 dB
PL13	17.70 dB
SF02	500.0355000 MHz
SI	32768
SF	125.7326442 MHz
WDW	EM
SSB	0
LB	10.00 Hz
GB	0
PC	2.00

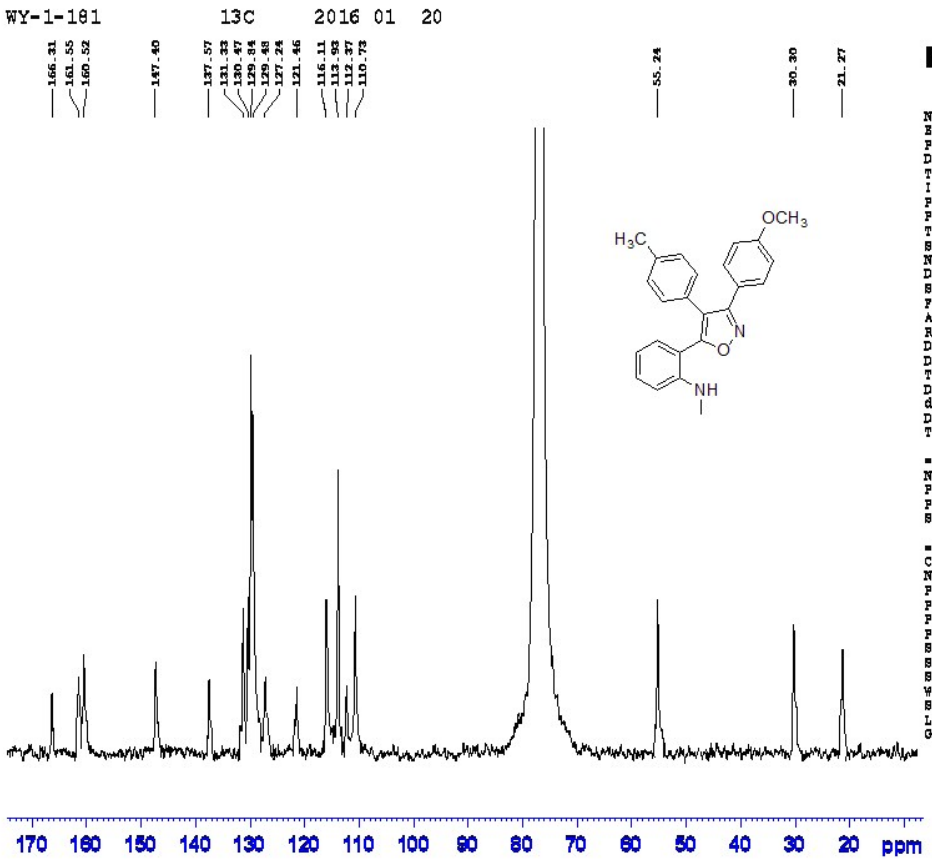
[1]H NMR Spectrum of 4p



BRUKER

NAME	WY-1-181
EXPNO	11
PROCNO	1
Date_	20140916
Time	17.54
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	16384
SOLVENT	CDCl3
NS	36
DS	1
SWH	10000.000 Hz
FIDRES	0.610352 Hz
AQ	0.8193000 sec
RG	912
DW	50.000 usec
DE	8.00 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.00 usec
PL1	2.00 dB
SFO1	500.0338500 MHz
SI	16384
SF	500.0300120 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	5.00

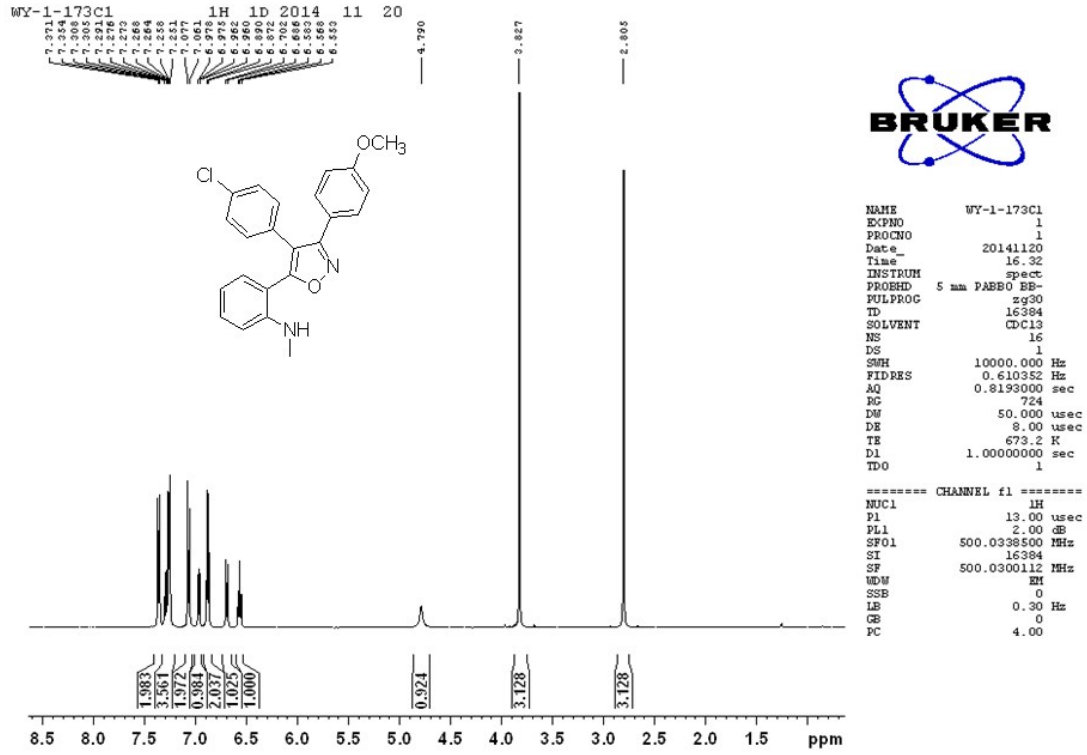
[13]C NMR Spectrum of 4p



BRUKER

NAME	WY-1-181
EXPNO	2
PROCNO	1
Date_	20160120
Time	15.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	5256
DS	2
SWH	32679.738 Hz
FIDRES	0.498653 Hz
AQ	1.0027661 sec
RG	367
DW	15.300 usec
DE	6.00 usec
TE	673.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	40
======== CHANNEL f1 ========	
NUC1	13C
P1	12.20 usec
PL1	3.00 dB
SFO1	125.7464750 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	17.70 dB
PL13	17.70 dB
SFO2	500.0355000 MHz
SI	32768
SF	125.7326420 MHz
WDW	EM
SSB	0
LB	26.00 Hz
GB	0
	2.00

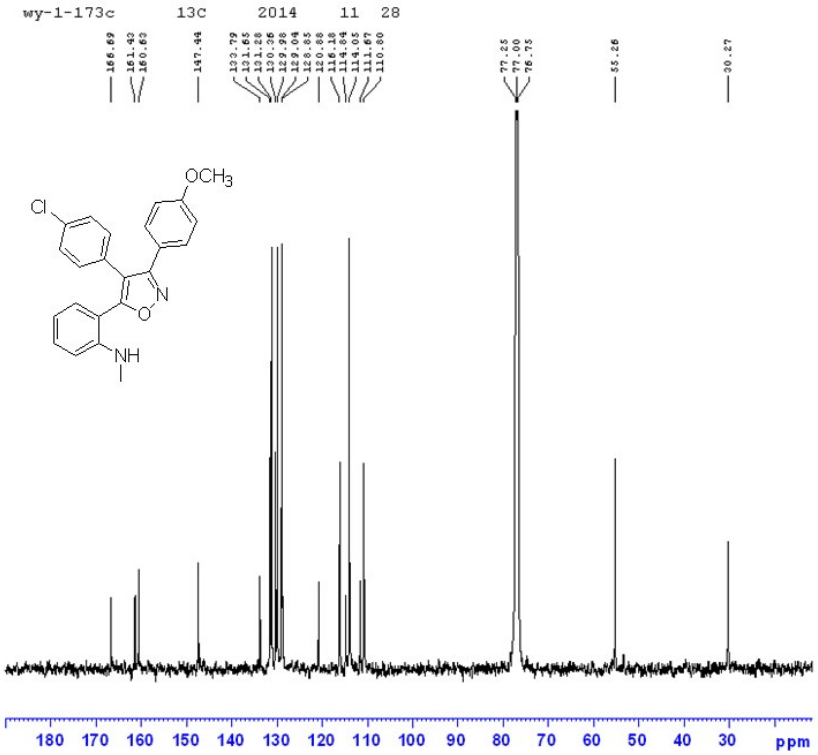
^{1}H NMR Spectrum of 4q



BRUKER

NAME	WY-1-173C1
EXPNO	1
PROCNO	1
Date_	20141120
Time	16.32
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	16384
SOLVENT	CDCl3
NS	16
DS	1
SWH	10000.000 Hz
FIDRES	0.610352 Hz
AQ	0.8193000 sec
RG	724
DW	50.000 usec
DE	8.00 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.00 usec
PL1	2.00 dB
SF01	500.0338500 MHz
SI	16384
SF	500.0300112 MHz
WDW	EM
SSB	0
LB	0.30 Hz
GB	0
PC	4.00

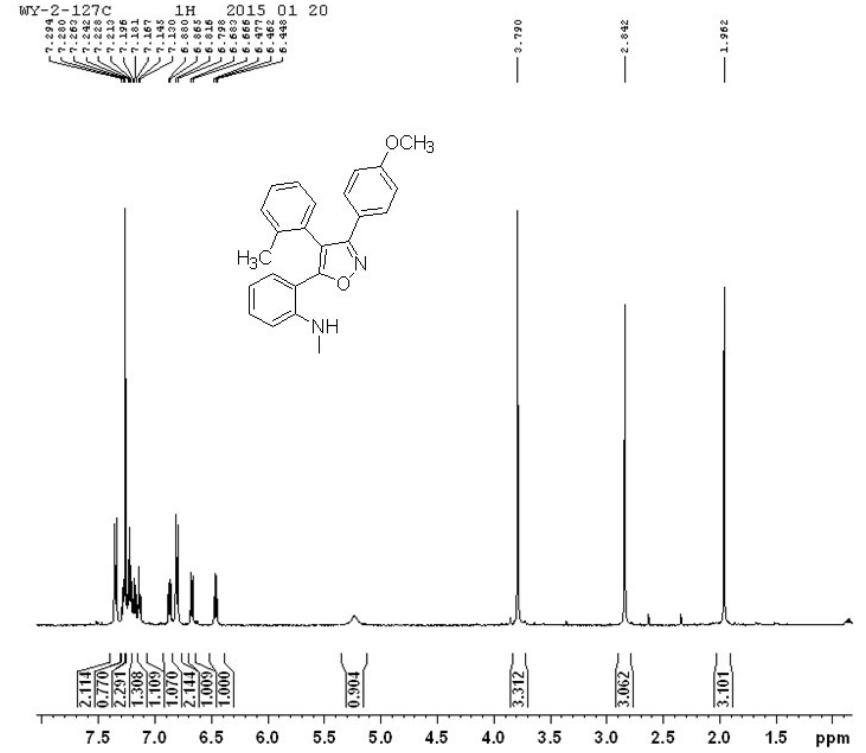
^{13}C NMR Spectrum of 4q



BRUKER

NAME	WY-1-173C1
EXPNO	2
PROCNO	1
Date_	20141128
Time	16.24
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	2974
DS	2
SWH	32679.738 Hz
FIDRES	0.498653 Hz
AQ	1.0027661 sec
RG	2580
DW	15.300 usec
DE	6.00 usec
TE	673.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	40
======== CHANNEL f1 ========	
NUC1	13C
P1	12.20 usec
PL1	3.00 dB
SF01	125.7464750 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	17.70 dB
PL13	17.70 dB
SF02	500.0355000 MHz
SI	32768
SF	125.7326476 MHz
WDW	EM
SSB	0
LB	8.00 Hz
GB	0
PC	2.00

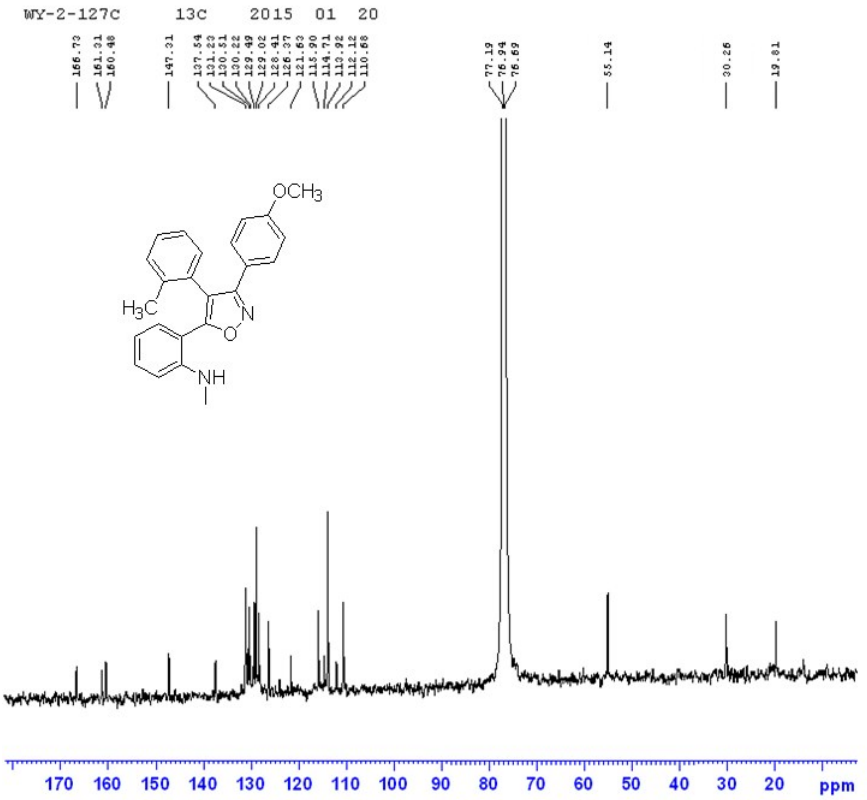
^{1}H NMR Spectrum of 4r



```
NAME            WY-2-127C
EXPNO                   1
PROCNO                  1
Date_            20150120
Time                17.50
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      1
SWH             10000.000 Hz
FIDRES              0.305176 Hz
AQ                1.6385000 sec
RG                    645
DW                 50.000 usec
DE                  6.00 usec
TE                 673.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  13.00 usec
PL1                  2.00 dB
SF01          500.0335010 MHz
SI                  16384
SF            500.0300091 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   4.00
```

^{13}C NMR Spectrum of 4r

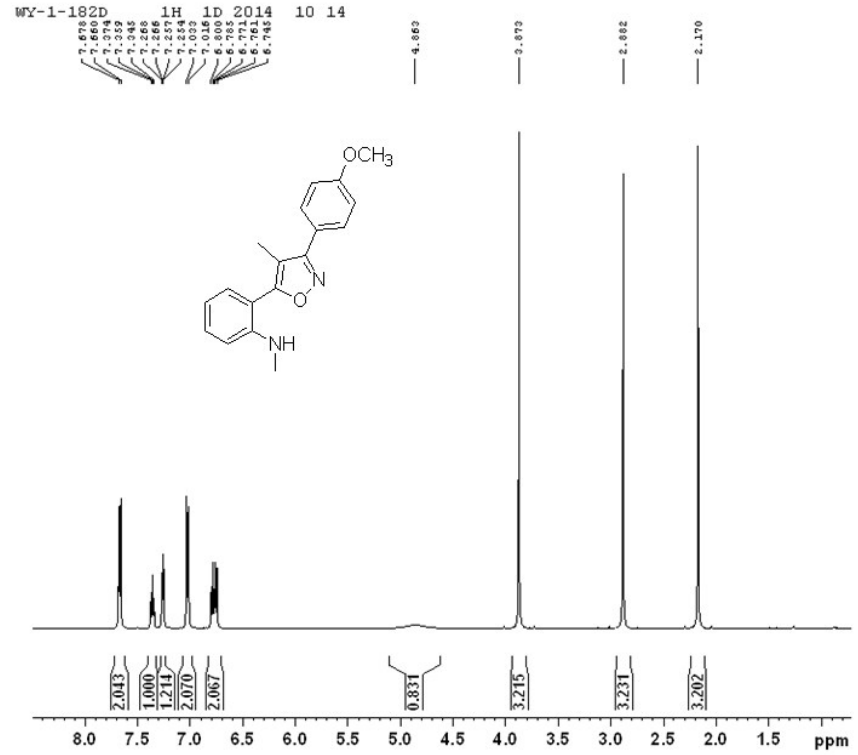


```
NAME            WY-2-127C
EXPNO                   2
PROCNO                  1
Date_            20150120
Time                21.46
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                  12127
DS                      2
SWH             32679.738 Hz
FIDRES              0.498653 Hz
AQ                1.0027661 sec
RG                   1820
DW                 15.300 usec
DE                  6.00 usec
TE                 673.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                    20

======== CHANNEL f1 ========
NUC1                  13C
P1                  12.20 usec
PL1                  3.00 dB
SF01          125.7464750 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  2.00 dB
PL12                17.70 dB
PL13                17.70 dB
SF02          500.0355000 MHz
SI                  32768
SF            125.7326512 MHz
WDW                    EM
SSB                     0
LB                  12.00 Hz
GB                      0
PC                   1.00
```

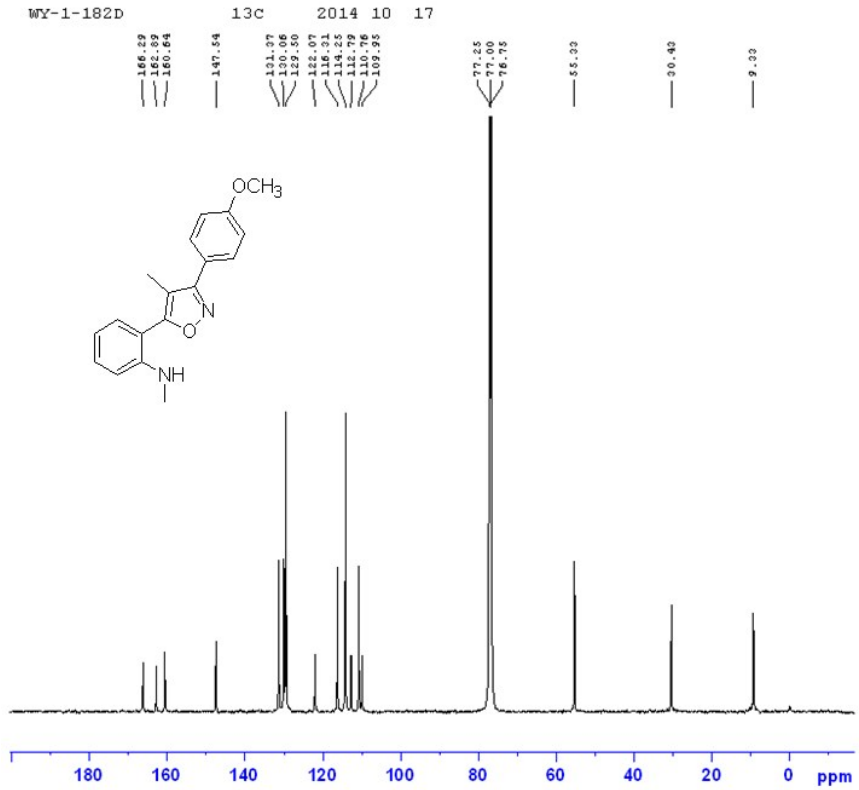
^{1}H NMR Spectrum of 4s



BRUKER

NAME	WY-1-182D
EXPNO	11
PROCNO	1
Date_	20141014
Time	14.21
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zg30
TD	16384
SOLVENT	CDCl3
NS	16
DS	1
SWH	10000.000 Hz
FIDRES	0.610352 Hz
AQ	0.8193000 sec
RG	912
DW	50.000 usec
DE	8.00 usec
TE	673.2 K
D1	1.00000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	1H
P1	13.00 usec
PL1	2.00 dB
SFO1	500.0338500 MHz
SI	16384
SF	500.0300120 MHz
WDW	EM
SSB	0
LB	0.50 Hz
GB	0
PC	5.00

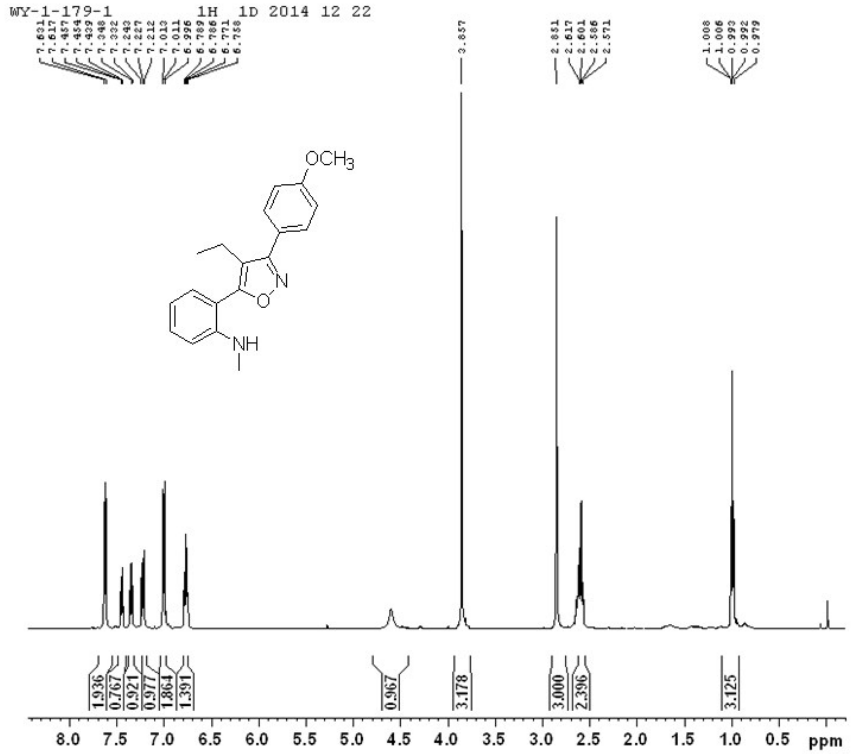
^{13}C NMR Spectrum of 4s



BRUKER

NAME	WY-1-182D
EXPNO	2
PROCNO	1
Date_	20141017
Time	22.14
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	13607
DS	2
SWH	32679.738 Hz
FIDRES	0.498653 Hz
AQ	1.0027661 sec
RG	3250
DW	15.300 usec
DE	6.00 usec
TE	673.2 K
D1	2.00000000 sec
d11	0.03000000 sec
DELTA	1.89999998 sec
TD0	40
======== CHANNEL f1 ========	
NUC1	13C
P1	12.20 usec
PL1	3.00 dB
SFO1	125.7464750 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	2.00 dB
PL12	17.70 dB
PL13	17.70 dB
SFO2	500.0355000 MHz
SI	32768
SF	125.7326441 MHz
WDW	EM
SSB	0
LB	12.00 Hz
GB	0
PC	2.00

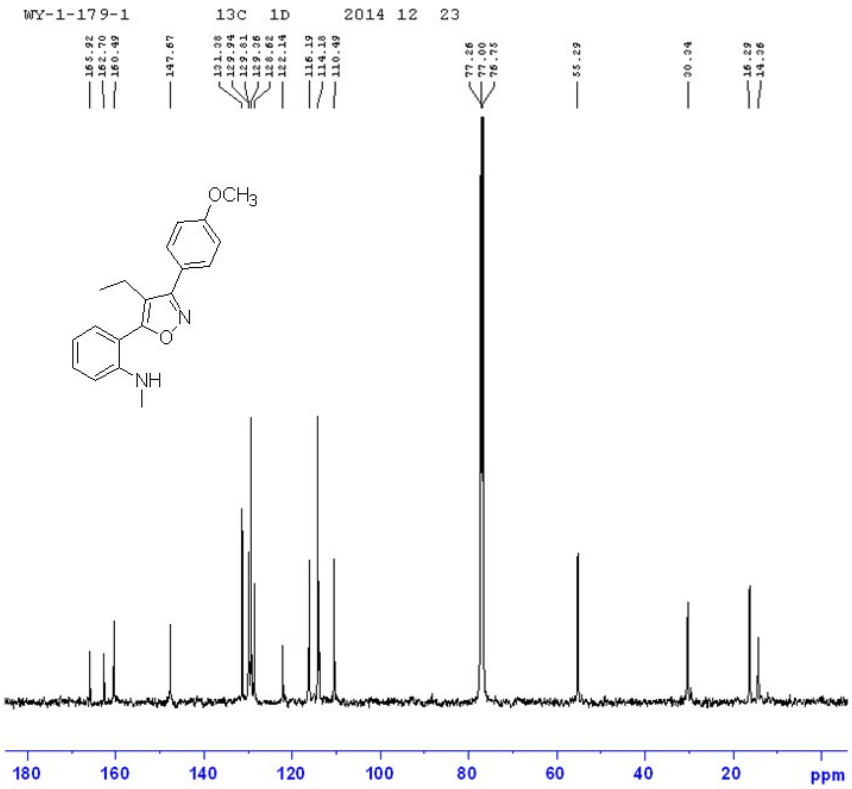
[1]H NMR Spectrum of 4t




```
NAME            WY-1-179
EXPNO                1
PROCNO               1
Date_         20141222
Time             16.38
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG           zg30
TD               16384
SOLVENT          CDCl3
NS                   8
DS                   1
SWH          10000.000 Hz
FIDRES        0.610352 Hz
AQ            0.8193000 sec
RG                 144
DW              50.000 usec
DE               8.00 usec
TE              673.2 K
D1           1.00000000 sec
TD0                  1

======== CHANNEL f1 ========
NUC1               1H
P1              13.00 usec
PL1              2.00 dB
SFO1       500.0338500 MHz
SI               16384
SF         500.0300192 MHz
WDW                EM
SSB                 0
LB              0.30 Hz
GB                  0
PC              2.00
```

[13]C NMR Spectrum of 4t

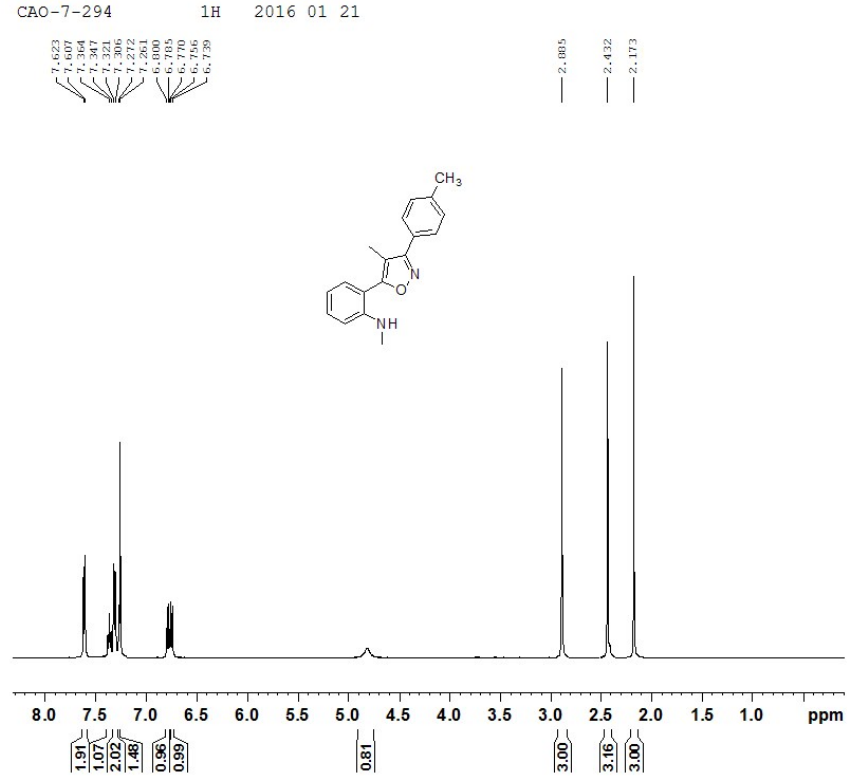



```
NAME            WY-1-179
EXPNO                2
PROCNO               1
Date_         20141223
Time             15.44
INSTRUM          spect
PROBHD   5 mm PABBO BB-
PULPROG        zgpg30
TD               65536
SOLVENT          CDCl3
NS                 705
DS                   2
SWH          32679.738 Hz
FIDRES        0.498653 Hz
AQ            1.0027661 sec
RG                1820
DW              15.300 usec
DE               6.00 usec
TE              673.2 K
D1           2.00000000 sec
D11          0.03000000 sec
DELTA        1.89999998 sec
TD0                 20

======== CHANNEL f1 ========
NUC1               13C
P1              12.20 usec
PL1              3.00 dB
SFO1       125.7464750 MHz

======== CHANNEL f2 ========
CPDPRG2         waltz16
NUC2               1H
PCPD2           80.00 usec
PL2              2.00 dB
PL12            17.70 dB
PL13            17.70 dB
SFO2       500.0355000 MHz
SI               32768
SF         125.7326512 MHz
WDW                EM
SSB                 0
LB              10.00 Hz
GB                  0
PC              1.00
```

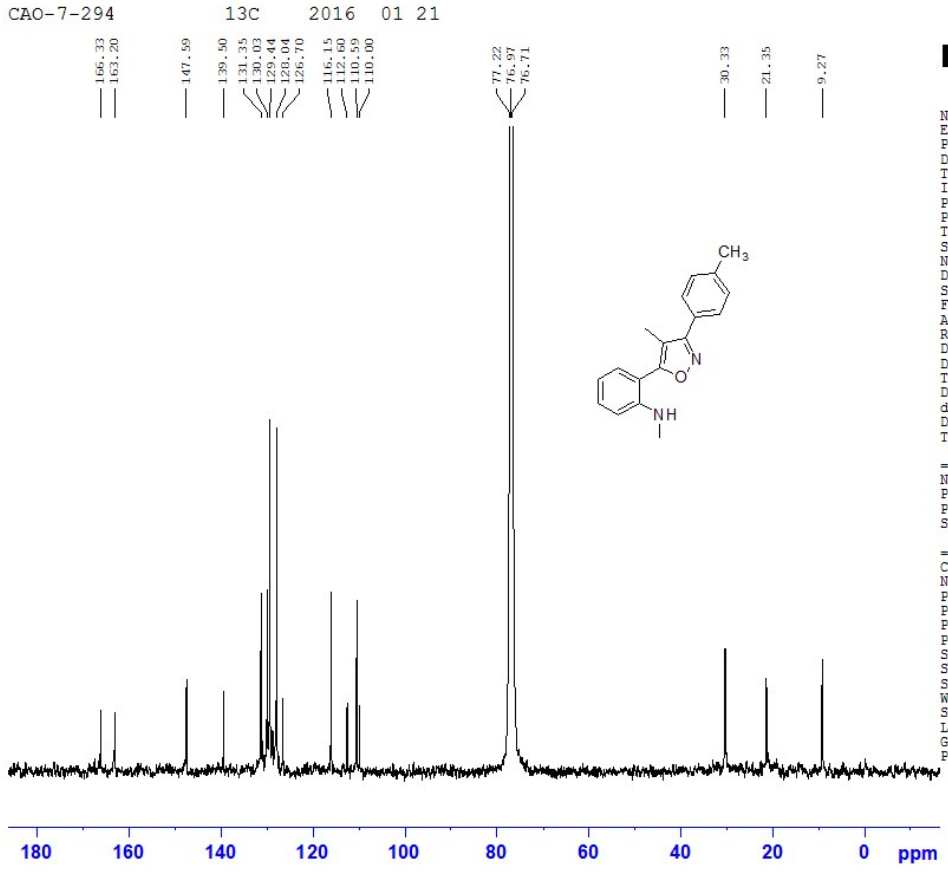
[1]H NMR Spectrum of 4u




```
NAME          CAO-7-294
EXPNO                 1
PROCNO                1
Date_          20160121
Time              15.29
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG            zg30
TD                32768
SOLVENT           CDCl3
NS                   16
DS                    1
SWH           10000.000 Hz
FIDRES        0.305176 Hz
AQ            1.6385000 sec
RG                  812
DW               50.000 usec
DE                6.00 usec
TE               673.2 K
D1            2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 1H
P1                13.00 usec
PL1                2.00 dB
SFO1         500.0335010 MHz
SI                16384
SF           500.0300097 MHz
WDW                  EM
SSB                   0
LB                0.30 Hz
GB                    0
PC                4.00
```

[13]C NMR Spectrum of 4u

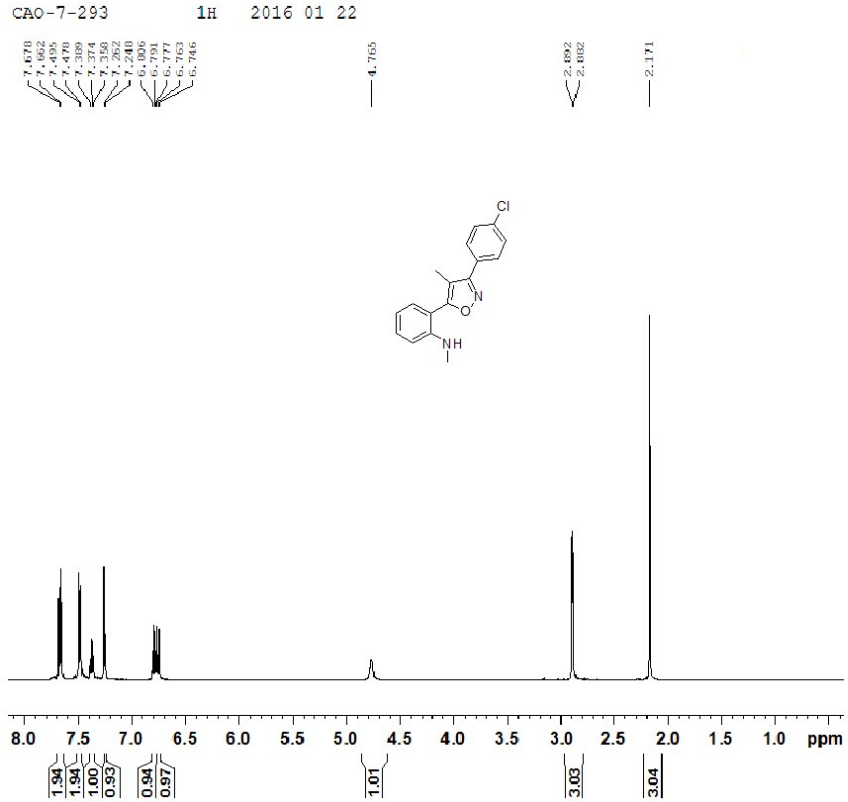



```
NAME          CAO-7-294
EXPNO                 2
PROCNO                1
Date_          20160121
Time              22.57
INSTRUM           spect
PROBHD   5 mm PABBO BB-
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                13506
DS                    2
SWH           32679.738 Hz
FIDRES        0.498653 Hz
AQ            1.0027661 sec
RG                 3640
DW               15.300 usec
DE                6.00 usec
TE               673.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                  20

======== CHANNEL f1 ========
NUC1                13C
P1                12.20 usec
PL1                3.00 dB
SFO1        125.7464750 MHz

======== CHANNEL f2 ========
CPDPRG2          waltz16
NUC2                 1H
PCPD2             80.00 usec
PL2                2.00 dB
PL12              17.70 dB
PL13              17.70 dB
SFO2         500.0355000 MHz
SI                32768
SF          125.7326487 MHz
WDW                  EM
SSB                   0
LB               10.00 Hz
GB                    0
PC                1.00
```

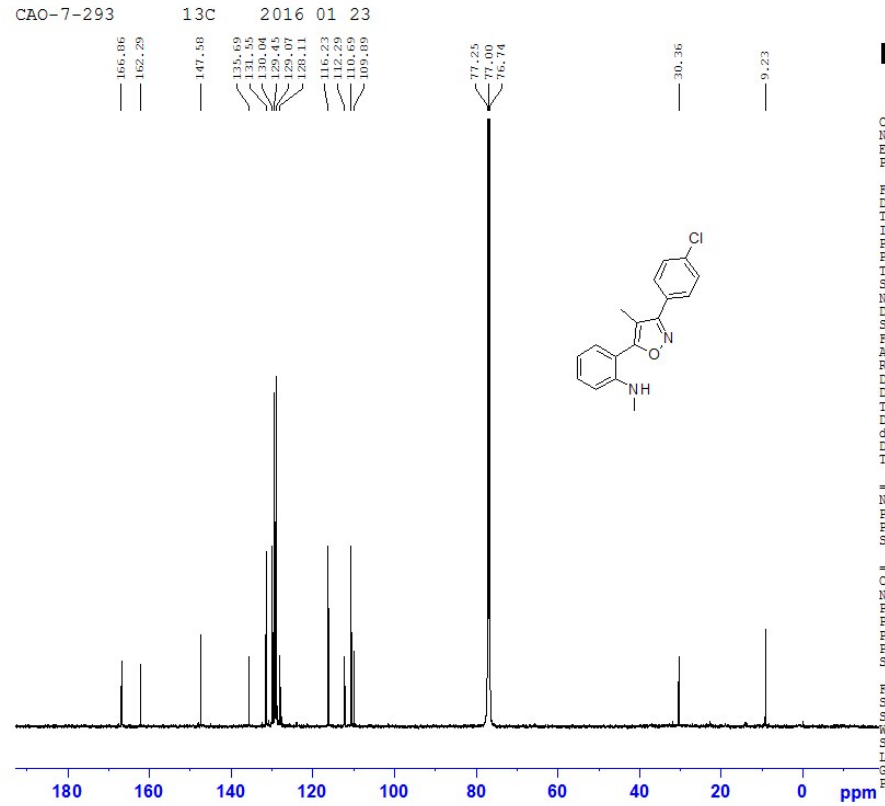
[1]H NMR Spectrum of 4v




```
NAME            CAO-7-293
EXPNO                   1
PROCNO                  1
Date_            20160122
Time                17.34
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      1
SWH             10000.000 Hz
FIDRES          0.305176 Hz
AQ              1.6385000 sec
RG                    812
DW                50.000 usec
DE                 6.00 usec
TE                673.2 K
D1              2.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 13.00 usec
PL1                 2.00 dB
SFO1          500.0335010 MHz
SI                  16384
SF            500.0300097 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 4.00
```

[13]C NMR Spectrum of 4v




```
Current Data Parameters
NAME            CAO-7-293
EXPNO                   2
PROCNO                  1

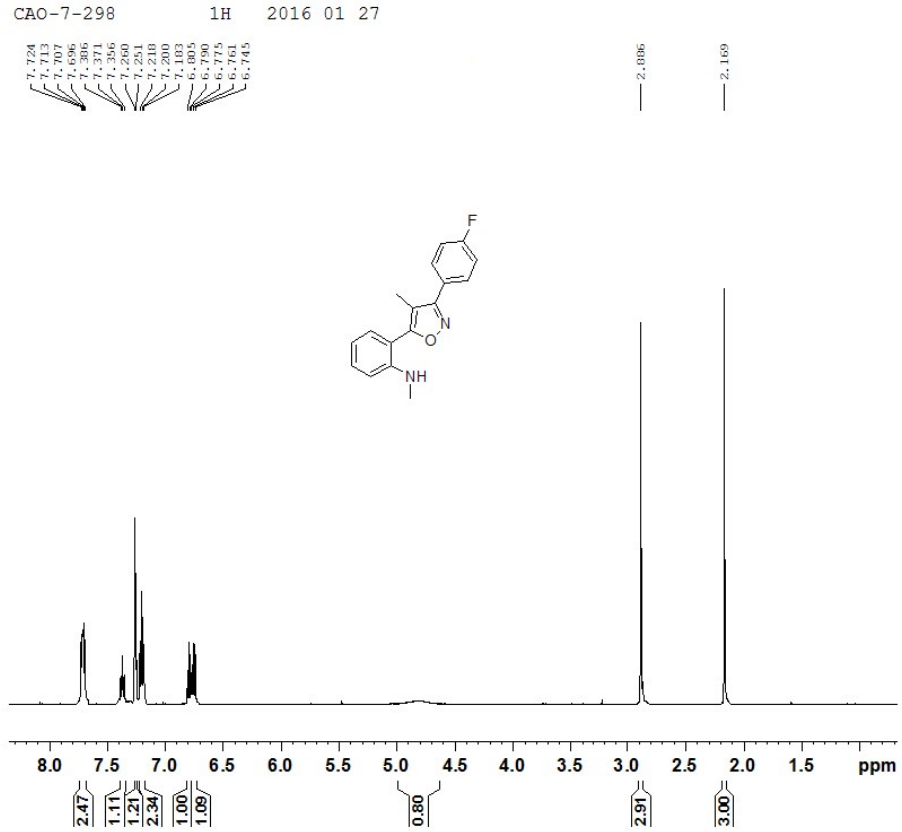
F2 - Acquisition Parameters
Date_            20160123
Time                21.11
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                  20000
DS                      2
SWH             32679.738 Hz
FIDRES          0.498653 Hz
AQ              1.0027661 sec
RG                   2300
DW                15.300 usec
DE                 6.00 usec
TE                673.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                    20

======== CHANNEL f1 ========
NUC1                   13C
P1                 12.20 usec
PL1                 3.00 dB
SFO1          125.7464750 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 2.00 dB
PL12               17.70 dB
PL13               17.70 dB
SFO2          500.0355000 MHz

F2 - Processing parameters
SI                  32768
SF            125.7326469 MHz
WDW                    EM
SSB                     0
LB                 3.00 Hz
GB                      0
PC                 1.00
```

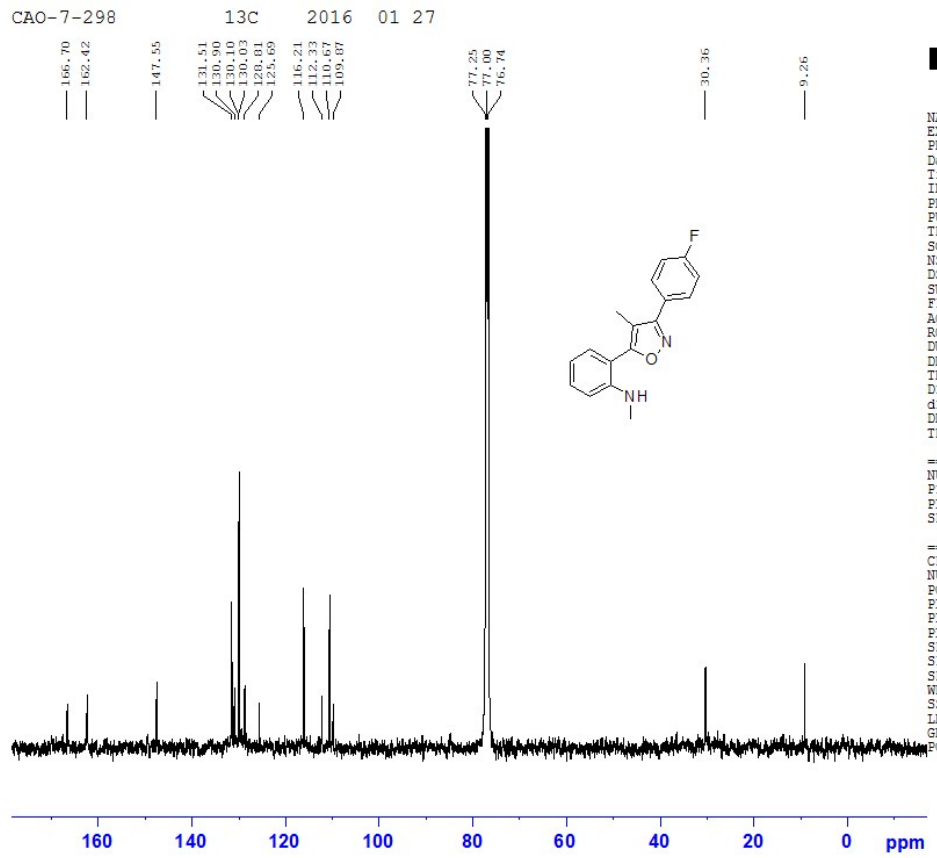
[1]H NMR Spectrum of 4w




```
NAME            CAO-7-298
EXPNO                   1
PROCNO                  1
Date_            20160127
Time                 9.57
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      1
SWH             10000.000 Hz
FIDRES          0.305176 Hz
AQ              1.6385000 sec
RG                    406
DW                50.000 usec
DE                 6.00 usec
TE                673.2 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                 13.00 usec
PL1                 2.00 dB
SFO1          500.0335010 MHz
SI                  16384
SF            500.0300102 MHz
WDW                    EM
SSB                     0
LB                 0.30 Hz
GB                      0
PC                 4.00
```

[13]C NMR Spectrum of 4w

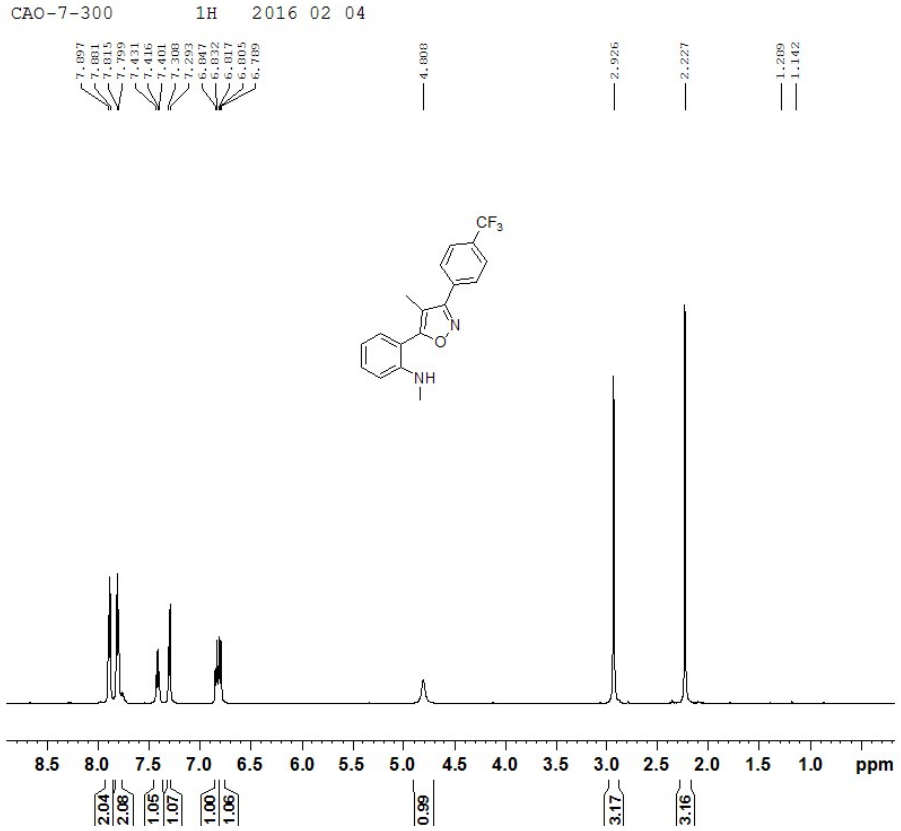



```
NAME            CAO-7-298
EXPNO                   2
PROCNO                  1
Date_            20160127
Time                13.28
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   2281
DS                      2
SWH            32679.738 Hz
FIDRES          0.498653 Hz
AQ              1.0027661 sec
RG                   3640
DW                15.300 usec
DE                 6.00 usec
TE                673.2 K
D1            2.00000000 sec
d11           0.03000000 sec
DELTA         1.89999998 sec
TD0                    20

======== CHANNEL f1 ========
NUC1                  13C
P1                 12.20 usec
PL1                 3.00 dB
SFO1         125.7464750 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2              80.00 usec
PL2                 2.00 dB
PL12               17.70 dB
PL13               17.70 dB
SFO2          500.0355000 MHz
SI                  32768
SF           125.7326487 MHz
WDW                    EM
SSB                     0
LB                 6.00 Hz
GB                      0
PC                 1.00
```

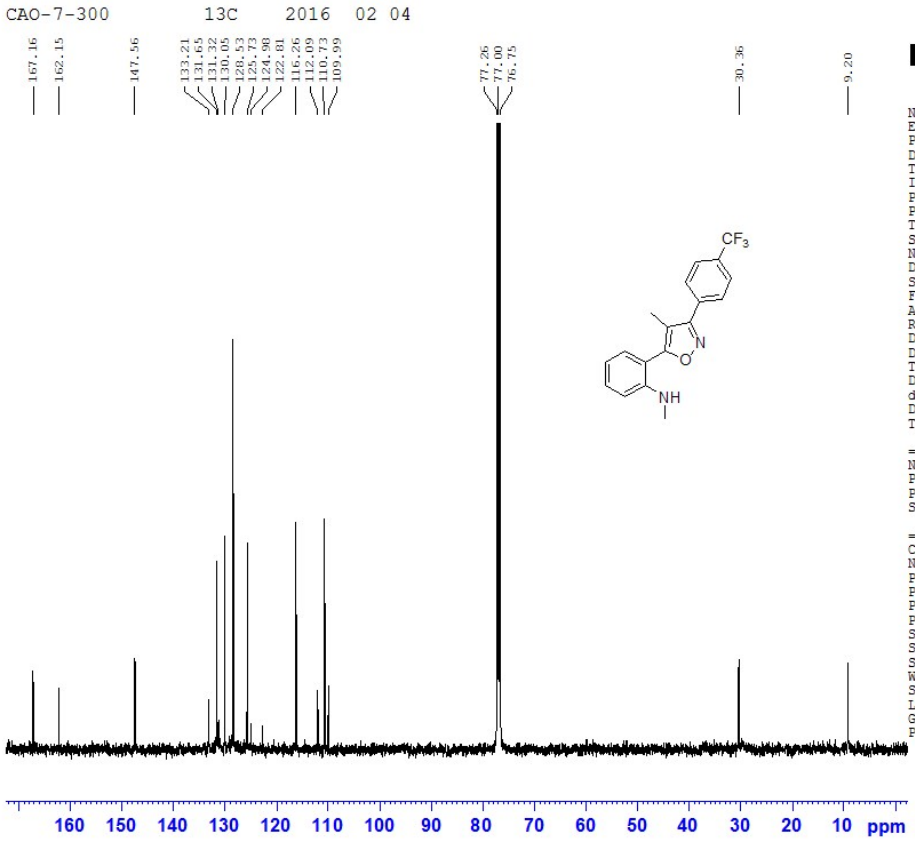
^{1}H NMR Spectrum of 4x



```
NAME            CAO-7-300
EXPNO                   1
PROCNO                  1
Date_            20160204
Time                12.31
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG              zg30
TD                  32768
SOLVENT             CDCl3
NS                      8
DS                      1
SWH             10000.000 Hz
FIDRES              0.305176 Hz
AQ              1.6385000 sec
RG                    228
DW                 50.000 usec
DE                  6.00 usec
TE                 673.2 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  13.00 usec
PL1                  2.00 dB
SFO1          500.0335010 MHz
SI                  16384
SF            500.0299937 MHz
WDW                    EM
SSB                     0
LB                   0.30 Hz
GB                      0
PC                   4.00
```

^{13}C NMR Spectrum of 4x



```
NAME            CAO-7-300
EXPNO                   2
PROCNO                  1
Date_            20160204
Time                12.47
INSTRUM             spect
PROBHD    5 mm PABBO BB-
PULPROG           zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    500
DS                      2
SWH             32679.738 Hz
FIDRES              0.498653 Hz
AQ              1.0027661 sec
RG                   3640
DW                 15.300 usec
DE                  6.00 usec
TE                 673.2 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                    20

======== CHANNEL f1 ========
NUC1                  13C
P1                  12.20 usec
PL1                  3.00 dB
SFO1         125.7464750 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                   1H
PCPD2               80.00 usec
PL2                  2.00 dB
PL12                17.70 dB
PL13                17.70 dB
SFO2          500.0355000 MHz
SI                  32768
SF            125.7326487 MHz
WDW                    EM
SSB                     0
LB                   3.00 Hz
GB                      0
PC                   1.00
```